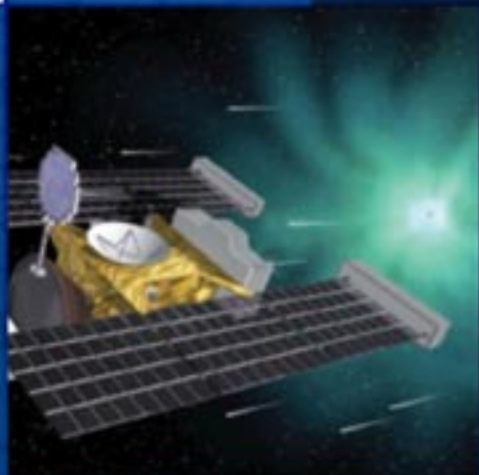
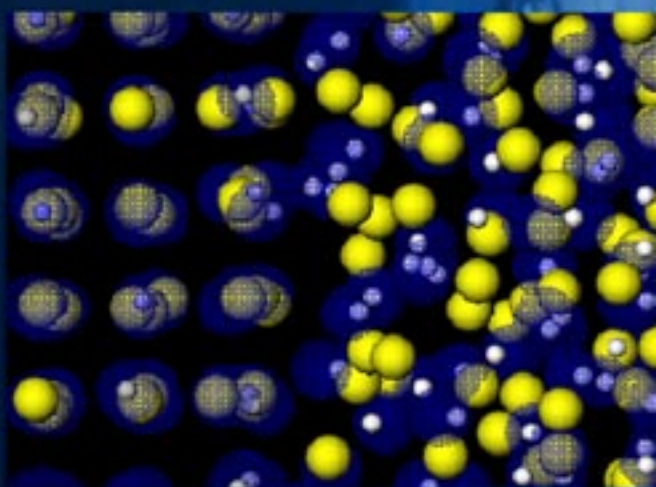
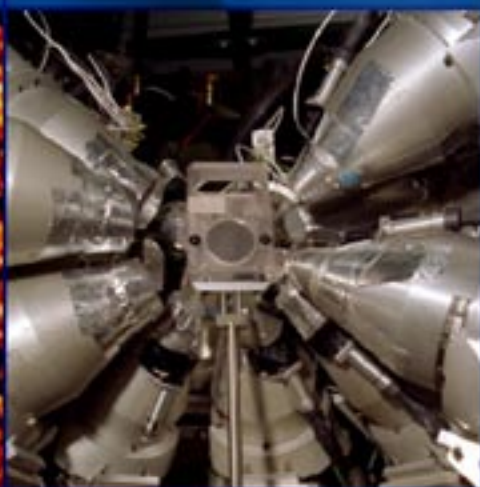




Physics and Advanced Technologies

LAWRENCE LIVERMORE NATIONAL LABORATORY



2003
ANNUAL
REPORT

ABOUT THE COVER

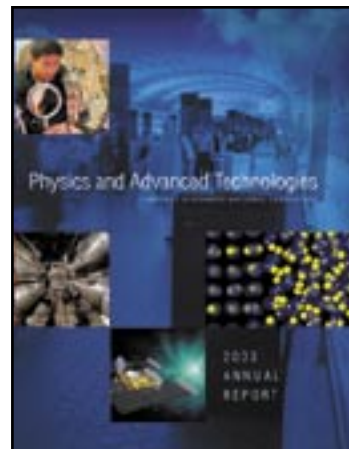
Background: Test deployment of the Autonomous Pathogen Detection System in a US subway, which was featured as the cover article of *Analytical Chemistry* on October 15, 2003. The Chemical Abstracts Service of the American Chemical Society selected this article, written by researchers from Livermore and the US Army Dugway Proving Grounds' West Desert Test Center, from a list of about 200,000 documents as the most intriguing paper of fourth quarter 2003.

Top Left: Scientist Prav Patel aligning a diagnostic in the JanUSP target chamber. JanUSP is one of the world's brightest ultrashort pulse lasers and used primarily for high-energy-density physics experiments in Physics and Advanced Technologies' Janus laser complex.

Middle Left: Gamma detector used to measure gamma rays emitted in neutron-induced nuclear reactions at the Los Alamos Neutron Science Center in New Mexico. Experimental results led to an accurate determination of nuclear reaction cross sections for plutonium-239 and other isotopes, which are important for interpreting past underground nuclear tests.

Middle Right: Representation of atoms from a first-principles, molecular dynamics simulation of the melting of lithium hydride. This particular configuration shows the interface between solid and liquid phases. Simulations of 432 atoms were made possible by theoretical and computational advances and Livermore's massively parallel computing capabilities supported by the National Nuclear Security Administration's Advanced Simulation and Computing Program.

Bottom: Artist rendition of the STARDUST spacecraft near the Comet Wild-2. Aerogel collectors were deployed to collect a dust sample from the comet as well as interstellar dust, which will greatly improve our understanding of the composition and abundance of elements in outer space. Samples have been stowed for return to Earth in February 2006.



Cover design: Amy Henke

ABOUT PHYSICS AND ADVANCED TECHNOLOGIES

The Physics and Advanced Technologies Directorate was established in July 2000 through the merger of the former Physics Directorate and elements of the former Laser Programs. The directorate has a budget of approximately \$160 million and a staff of approximately 350 employees. We are highly integrated and multidisciplinary, with substantive collaborations with the rest of Lawrence Livermore National Laboratory and with other national laboratories, universities, and industry. Our mission is to be a leader in frontier physics and technology for 21st-century national security missions: stockpile stewardship, homeland security, energy independence, and the exploration and use of space.

FIND OUT MORE ABOUT US

Visit our Web site at <http://www-pat.llnl.gov/> for more information on Physics and Advanced Technologies research, facilities, publications, staff, organization, events, and awards.

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CONTENTS

Introduction	2
Signature Experimental Facilities	4
High-Energy-Density Physics and Astrophysics Division	8
Condensed Matter Physics Division	16
Nuclear, Particle, and Accelerator Physics Division	24
Institute of Geophysics and Planetary Physics	32
Optical Science and Technology Division	38
Institute for Laser Science and Applications	46
Medical Physics and Biophysics Division	52
Fusion Energy Program	60
Physics and Advanced Technologies Awards	72

INTRODUCTION



William H. Goldstein
Associate Director, Physics
and Advanced Technologies
Directorate

The Physics and Advanced Technologies (PAT) Directorate overcame significant challenges in 2003 to deliver a wealth of scientific and programmatic milestones, and move toward closer alignment with programs at Lawrence Livermore National Laboratory.

We acted aggressively in enabling the PAT Directorate to contribute to future, growing Lawrence Livermore missions in homeland security and at the National Ignition Facility (NIF). We made heavy investments to bring new capabilities to the Laboratory, to initiate collaborations with major Laboratory programs, and to align with future Laboratory directions. Consistent with our mission, we sought to ensure that Livermore programs have access to the best science and technology, today and tomorrow.

For example, in a move aimed at revitalizing the Laboratory's expertise in nuclear and radiation detection, we brought the talented Measurement Sciences Group to Livermore from Lawrence Berkeley National Laboratory, after its mission there had diminished. The transfer to our I Division entailed significant investment by PAT in equipment and infrastructure required by the group. In addition, the move occurred at a time when homeland security funding was expected, but not yet available. By the end of the year, though, the group was making crucial contributions to the radiation detection program at Livermore, and nearly every member was fully engaged in programmatic activities.

Our V Division made a move of a different sort, relocating en masse from Building 121 to the NIF complex. This move was designed to enhance interaction and collaboration among

high-energy-density experimental scientists at the Laboratory, a goal that is essential to the effective use of NIF in the future. Since then, V Division has become increasingly integrated with NIF activities. Division scientists are heavily involved in diagnostic development and fielding and are poised to perform equation-of-state and high-temperature hohlraum experiments in 2004 as part of the NIF Early Light program.

In reviewing the major scientific and programmatic results from PAT that are elaborated in this report, it's not surprising to find many that are the result of investments made in world-class scientific capability over the past years. For example, in 2003 our scientists

- Commissioned a new high-pressure research facility at the Advanced Photon Source and used it to experimentally confirm for the first time the high-pressure phase diagram of plutonium.
- Executed the first two experiments at the Joint Actinide Shock Physics Experimental Research (JASPER) facility, obtaining plutonium equation-of-state data of unprecedented accuracy.
- Demonstrated the ability to focus ultrashort pulse, laser-produced proton beams and used the focused beam to heat matter isochorically. This work was recognized by *Physical Review Focus* for its potential to experimentally explore new states of matter.
- Established the capability to reproducibly produce intense, tunable picosecond pulses of hard x rays at the PLEIADES facility, an enabling development for dynamic materials experiments.

- Reduced the computing time for the hardest photon transport calculations by up to six orders of magnitude.
- Completed the adaptive optics system at the Keck Observatory and used it to image the merger of two galaxies with resolution better than the space telescope.
- Demonstrated in the laboratory the mechanism by which comets produce x rays, thereby resolving an outstanding controversy, as reported in *Science*.
- Won three R&D 100 awards.
- Developed an adaptive optics-based system to improve early diagnosis and treatment of retinal diseases.
- Devised a system to discriminate strains of closely related pathogens in a single sample.
- Understood nuclear reactions around black holes, relevant to gamma-ray bursts.
- Built the world's largest diffractive lens.

The PAT Directorate has extended its record of engagement and recognition in the scientific community, producing 430 refereed publications in 2003, including 3 in *Nature*, 3 in *Science*, and 39 in *Physical Review Letters*. Two PAT scientists were named fellows of the American Physical Society (APS), bringing the total to 46 in the directorate, and 2 others received APS awards.

Many recent developments will have ongoing impact on the PAT Directorate and its mission. Lawrence Livermore has completed the first round of long-range science and technology planning and has started to use the plan as a guide to science and technology investments Laboratory-wide. The plan recognizes and subsumes many of the themes and initiatives that PAT has pursued.

The Department of Energy (DOE) Office of Science plan for facility investments over the next 20 years was announced recently and includes, as the highest priorities, projects with significant PAT involvement. The Department of Homeland Security released significant science and technology funding, and Lawrence Livermore—with help from PAT—garnered disproportionate shares of efforts for countering nuclear terrorism and bioterrorism. Total support to PAT from the Nonproliferation, Arms Control, and International Security Directorate, including Homeland Security programs, doubled this year.

In a departure from past practice, DOE has decided to compete the management contracts for Los Alamos and Livermore (and other) national laboratories, adding uncertainty to the future. A zero-tolerance environment for mistakes presents new challenges for maintaining a robust research and development program that encourages work at the boundaries of knowledge. It often seems that the programs are asked to do more with less, leading to stress on longer-range research and the goal of scientific excellence.

We look forward to our first experiments on NIF in 2004 and development of full stockpile stewardship experimental programs at JASPER and the new high-pressure physics beamline at the Advanced Photon Source. We are counting on new counterterrorism capabilities that will be deployed, based on contributions of PAT scientists. And I am confident that the research underlying these advances will continue to receive the recognition and high regard of the scientific community.



Facilities

SIGNATURE EXPERIMENTAL FACILITIES

Experimental research constitutes a core activity in the Physics and Advanced Technologies (PAT) Directorate. We conduct experiments using a wide range of facilities, some at Lawrence Livermore National Laboratory and some at other research centers. As part of our commitment to maintaining a strong experimental science base at Lawrence Livermore, we operate several special facilities in support of Laboratory programs and its basic science mission.

The **Janus laser complex** houses two lasers in close proximity to one another: the long-pulse Janus laser, with two beams delivering up to 1000 joules of energy in 3 nanoseconds, and the Janus-pumped ultrashort-pulse laser, called JanUSP, which is one of the world's brightest, delivering 10 joules of energy on target with intensities higher than 10^{21} watts per square centimeter. Together, these lasers provide a platform for high-energy-density (HED) plasma physics and materials science experiments; for development, calibration, and testing of diagnostics for use on larger lasers such as the National Ignition Facility; and for recruiting and training HED scientists. An intense short-pulse (ISP) laser upgrade is under construction in the Janus laser complex. It will be capable of producing a few hundred joules of energy in a few picoseconds and will allow creation of high-energy K_{α} radiation and megaelectronvolt (MeV) proton beams for radiography. Adjacent to the Janus complex are two other smaller lasers: the three-beam picosecond COMET laser used primarily for x-ray laser research, and another ultrashort-pulse laser. In 2003, the entire laser facility supported experimental campaigns by 95 principal investigators, collaborators, and students from Lawrence Livermore and other institutions.

The **Lawrence Livermore gas-gun facility** is a premier shock physics facility used to create and study matter under a wide range of dynamic loading conditions that simulate weapons conditions. It houses two fully instrumented, two-stage, light-gas guns that can launch centimeter-sized projectiles at speeds up to 8 kilometers



The two-beam JANUS laser



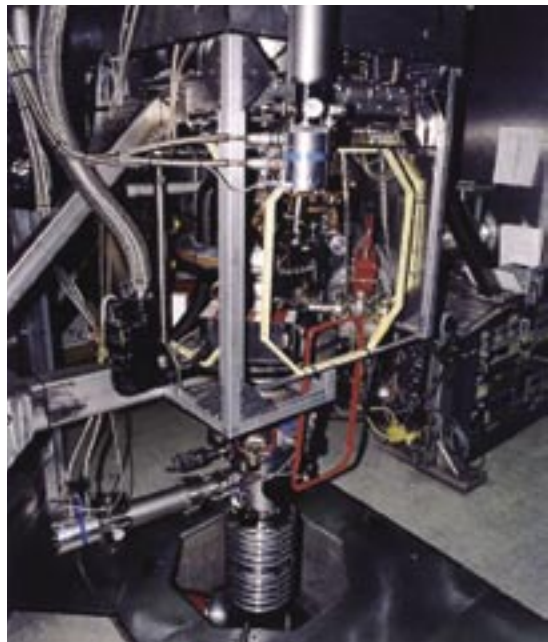
Two-stage gas-gun in Lawrence Livermore's shock physics facility

per second. The facility primarily supports experiments on materials at high pressures and temperatures to generate equation-of-state and material strength data. It also serves as a testbed for developing techniques and training personnel for experiments at the JASPER (Joint Actinide Shock Physics Experimental Research) facility at the Nevada Test Site for the Stockpile Stewardship Program. The Livermore gas guns have helped unravel scientific puzzles in condensed matter physics, geophysics, and planetary science. In 1996, we produced metallic hydrogen for the first time and measured its electrical conductivity as a function of pressure.

100-MeV Electron Linear Accelerator



Electron Beam Ion Trap (SuperEBIT) in Building 194 spectroscopic facility



The **100-MeV Electron Linear Accelerator** supports two unique experimental capabilities for the Stockpile Stewardship Program and the Laboratory's basic science mission. The facility produces the most intense positron beam in the United States, suitable for positron microscopy for three-dimensional characterization of material defects at the microscale. It also provides the high-brightness electron beam required for the production of hard, monochromatic, ultrafast x rays via Thomson scattering. The x-ray pulses are generated by the interaction of the electron beam with short bursts of intense visible light from a laser that is synchronized with the accelerator. The x rays are suitable for radiography, diffraction, and spectroscopy experiments that can characterize dynamic processes in materials on picosecond timescales.

The **Electron Beam Ion Trap (EBIT) facility** is the preeminent spectroscopic facility in the US for the study of highly charged atomic ions—up to fully ionized uranium. It consists of the 100-kiloelectronvolt SuperEBIT machine, with a suite of spectroscopic instruments that spans the spectrum from the visible and ultraviolet to the soft and hard x-ray regions. This ion trap provides long-lived, low-density clouds of very highly charged ions that can be selectively ionized and excited by tuning the energy of the electron beam. The facility supports experiments in nuclear and atomic physics as well as plasma physics and space science and serves as a nationally recognized training ground for experimental scientists. For the Stockpile Stewardship Program, EBIT experiments generate atomic data essential for benchmarking nonequilibrium models of high-temperature plasmas. In 2003, the facility hosted experiments by Lawrence Livermore staff

and participating guest collaborators from more than a dozen institutions in the US, Canada, and Germany.

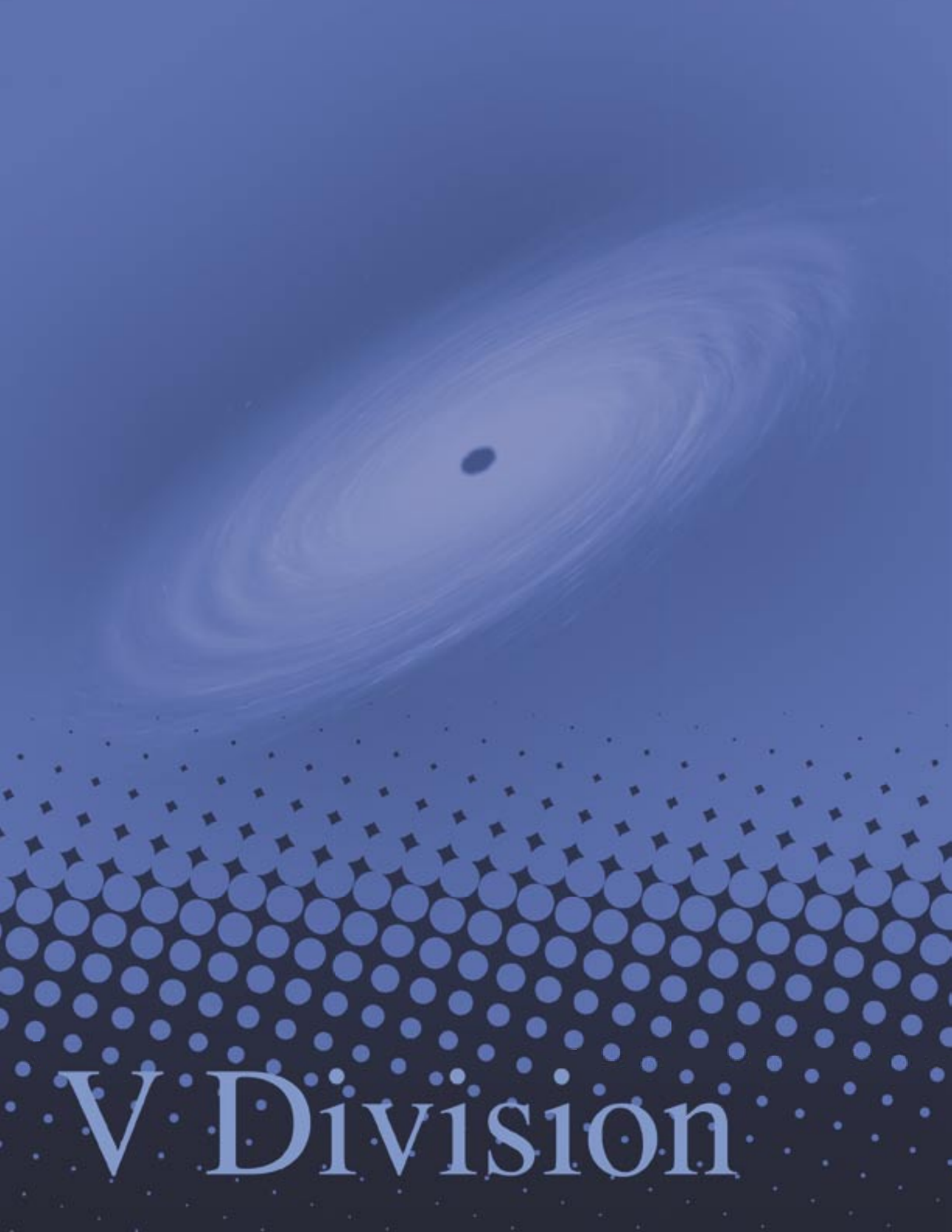
The **Spheromak** is a dedicated testbed for plasma physics experiments exploring a unique magnetic confinement geometry that is an alternative to tokamaks. The spheromak uses an internal dynamo to generate its confining magnetic field. The Livermore machine is equipped with a suite of advanced plasma diagnostics that researchers can use to investigate new magnetic configurations with unprecedented flexibility. The aim of the Sustained Spheromak Physics Experiment (SSPX) is to determine whether this confinement concept has sufficient promise for fusion energy to warrant a proof-of-principle fusion experiment. The facility also serves as a training ground for experimental plasma scientists and supports collaborations with faculty, postdoctoral scientists, and students from five institutions.

The **Experimental Test Accelerator-II (ETA-II)** is a 6-megaelectronvolt, 2-kiloampere, induction linear accelerator with a complete suite of beam and plasma diagnostics. The facility is ideally suited for experiments with intense electron beams. Originally, the facility was built as a high-average-power testbed for the Strategic Defense Initiative. Historically, ETA-II has been used as a driver for free electron lasers, as a radiation source for testing solid-state electronics, and for electron beam treatment of materials. In support of the Stockpile Stewardship Program, ETA-II is being used to develop bremsstrahlung x-ray targets capable of sustaining high doses for the DARHT-2 radiographic facility at Los Alamos National Laboratory. Other experiments at the facility involve the development and testing of new beam manipulation techniques and key hardware components for advanced radiographic missions.

Spheromak



Experimental Test Accelerator-II



V Division

HIGH-ENERGY-DENSITY PHYSICS AND ASTROPHYSICS DIVISION

The mission of the High-Energy-Density Physics and Astrophysics Division (known as V Division) is to advance understanding of the physical properties of matter at extreme conditions of temperature and density, where materials are significantly ionized into the plasma state.

The conditions range from temperatures of ten thousand degrees to hundreds of millions of degrees and pressures from a million atmospheres to many billions of atmospheres, spanning conditions from electrical sparks up to stellar interiors. The physical properties under study include radiative opacity, equations of state (EOS), and fundamental atomic spectroscopy and kinetics of high-temperature plasmas. These properties determine the creation, evolution, and energy balance of high-temperature plasmas. In addition, the spectra of the light emitted from plasmas, from visible up to x ray, provide an important method for diagnosing the conditions in plasmas far too hot to be measured by conventional in situ probes. Precise experimental measurements are used to develop and test advanced theoretical models for these plasma properties and processes. The models are incorporated into databases used by other programs, principally the Stockpile Stewardship Program and National Ignition Facility (NIF).

V Division's high-energy-density research program shares areas of common interest with astrophysics, including opacity, EOS, spectroscopy, development and use of radiation hydrodynamic simulation codes, and imaging and spectroscopic instrumentation. Because of these synergies, we undertake a collection of observational and computational astrophysics projects. These projects allow us to use astrophysical observations to constrain theoretical models, benefit from new developments in a large international community that shares many common interests, and recruit talented young scientists who have expertise in areas important to Laboratory programs.

The exotic temperature and pressure conditions described above are extremely difficult to produce in the laboratory. Ab initio theories of physical processes in these regimes are

also computationally intensive. We therefore use a number of unique facilities to conduct our research. These include high-energy laser facilities such as NIF, which recently began experimental operation with 4 of its eventual 192 beams. We also use the high-energy Omega laser facility operated by Rochester University. Other facilities include the large-scale pulsed-power machine (called "Z") at Sandia National Laboratory in Albuquerque, New Mexico, and high-intensity short-pulse lasers that produce very short-lived, very high-energy-density plasmas. On the computational side, our scientists use the massively parallel computer facilities sponsored by the Advanced Simulation and Computing Program.

Major V Division research activities of the past year are described in the following sections. Laboratory experimental facilities used during this research are described in the Signature Experimental Facilities section.

First-Generation, Detailed-Term-Accounting Opacity Code for Heavy Elements

Accurate descriptions of the transport, spectral emission, and EOS characteristics of equilibrium (LTE) and nonequilibrium (NLTE) plasmas are required for a number of Lawrence Livermore applications. These applications include nuclear weapons physics, design of LTE opacity experiments on platforms ranging from NIF to short-pulse lasers, and the assessment of NLTE radiative and electron transport effects in fast-ignition, high-intensity, x-ray backlighters and in x-ray free-electron-laser experiments. The analysis and computation of plasma opacities and EOS are particularly complex when there are large populations of ionic bound states.

In the LTE case, we use two approaches: (1) the detailed-term-accounting (DTA) scheme that explicitly computes the contributions of every significant transition, and (2) statistical treatments, such as super transition arrays that assemble an approximate model based on average properties of large spectral transition arrays. While the second approach has the advantage of speed, the detailed spectral models of the first approach are necessary

to evaluate the accuracy of the statistical methods and are known to be essential in some density and temperature regimes. Furthermore, assessment of proposed opacity experiments at NIF requires detailed spectral analysis because knowing the relative transparency of the spaces between the main spectral lines determines overall opacity.

V Division's OPAL code successfully demonstrated the importance of a DTA treatment for astrophysical problems involving open-M-shell iron, requiring serial calculations of about 1 to 100 million spectral lines. Extending the DTA treatment to heavier elements requires the parallel computation of trillions of lines and therefore needs many algorithmic innovations to be practicable [*Journal of Quantitative Spectroscopy and Radiative Transfer* **81**, 227 (2003)]. We have achieved spectacular speedups of the advanced DTA opacity code through a series of theoretical and computational developments, such as the application of a second quantized treatment of angular momentum algebra. The advanced opacity code, now being applied to computations for heavy elements, was selected as one of eight flagship projects to be given first access to the 128,000-processor BlueGene/L supercomputer in 2004. *Carlos Iglesias (iglesias1@llnl.gov)*

Opacity Experiments and High-Temperature Hohltraums

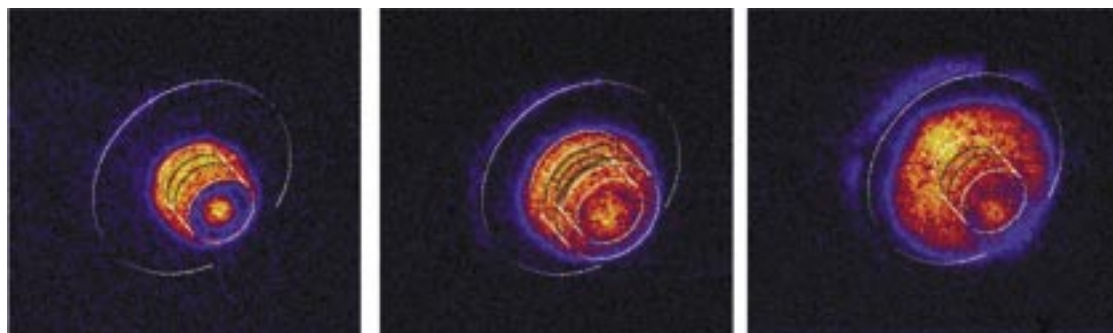
Radiative opacity experiments have been performed at temperatures slightly above 100 electronvolts (eV) using laser-driven hohltraums (hollow cylindrical enclosures) to generate x rays that uniformly heat sample materials. Laser energy is absorbed in the walls of a hohlraum made of a high-opacity (high-Z) material such as gold. Much of the laser

energy is converted to x rays that are emitted and reabsorbed by the walls of the enclosure, producing a high radiation field to heat the sample. Additional laser energy is used to produce a bright "backlighter" source of x rays. The attenuation of the backlighter x rays through the heated sample is used to measure the sample opacity.

The increased energy available on NIF will enable the production of hohltraums with much higher radiation temperatures. However, producing and using these high-energy-density regimes will require new experimental techniques and different target designs than previous experiments on Livermore's former Nova laser and the Omega laser.

The planned opacity experiments require a better understanding of the performance of high-temperature hohltraums, the development of new spectrometers and detectors, and the ability to produce backlighter sources that are brighter than the heated sample being probed. These hohltraums for opacity experiments are significantly outside the design parameters of the ignition hohltraums developed by the inertial confinement fusion (ICF) community. They are much smaller, hotter, and shorter lived, making the experiments more challenging. To understand the performance of these smaller, hotter hohltraums, we are conducting a series of scaled experiments at the Omega laser to investigate laser absorption and conversion to x rays, plasma filling and hole closure processes, and laser-plasma instabilities (Figure 1). In 2003, significant progress was made on measuring and ameliorating the effects of laser plasma instabilities that limit the amount of energy absorbed in these small targets. In addition, substantial improvements were made in the

1 Soft x-ray images of a small (400-micrometer-diameter) hollow cylindrical target heated by an external laser pulse. The images, taken at 300-picosecond intervals, show heating and expansion of the walls during the pulse (left to right). The rate of wall heating is dependent on the radiation temperature.



models used to predict the performance of these hohlraums.

In 2004, we will carry out experiments at the Omega laser to measure the opacity of gadolinium plasmas. Subsequently, these experiments will be extended to measure the opacity of materials used for radiation flow experiments. New spectrometers and rapidly gated, wide-field-of-view detectors, which are required to measure the opacity of short-lived, hot samples, are also under development. Research to develop and demonstrate bright, broadband, hohlraum-based backlighter sources has begun. Ultimately, these techniques will be transferred to NIF and scaled to opacity experiments at very high temperatures.

Marilyn Schneider (schneider5@llnl.gov)

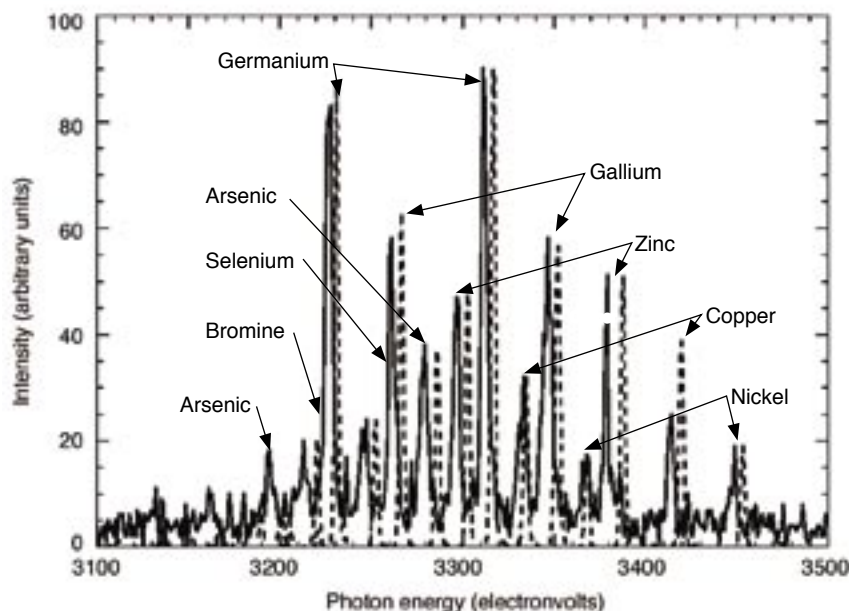
Ionization Balance of Nonequilibrium Gold Plasmas

High-energy-density physics experiments in the laboratory often use laser-heated gold hohlraum targets, as described above. The degree of ionization achieved in the laser-heated walls of the hohlraum determines the number of x rays produced and the amount of material ablated from the wall. Thus, it is important to have accurate models for the ionization balance of high-temperature gold plasmas. Experiments have been conducted at two facilities to investigate the physics that governs the ionization balance.

In experiments at the Omega laser, tamped gold samples were heated by direct laser illumination. The plasma electron temperature was measured by a Thomson scattering technique and by spectroscopy of tracer elements doped into the gold sample. The x-ray spectrum of gold in the 2.9 to 4 kiloelectronvolt (keV) range was used to estimate the charge state distribution of the gold plasma (Figure 2). The initial measurements were used to discriminate between different theoretical models for the ionization balance [*Physical Review Letters* **85**, 992 (2000)].

Subsequent experiments were conducted inside a hohlraum, and experimental parameters were varied to study the ionization balance as a function of the electron and radiation temperatures. The results show a strong variation with both electron temperature and radiation temperature when the electron temperature is below 1.5 keV, but relatively little variation with radiation temperature at higher electron temperatures. These experiments will be used to further discriminate between theoretical models and lend insight into the role of ionization and recombination processes under different conditions.

To better understand the complex physical processes that determine the ionization balance, we also conducted experiments at the Laboratory's Electron Beam Ion Trap (EBIT). EBIT allows greater control over the



2 The proportion of different charge states of highly ionized gold ions is determined by comparing the measured x-ray spectra to calculations of the emissivities of individual charge states.

plasma conditions, albeit at very low plasma density—about a billion times lower than in the laser experiments described above. At such low density, the plasma is in the coronal limit in which the ionization balance is independent of electron density. The experiments conducted in the two regimes emphasize different atomic processes and thus help to elucidate the role each plays in determining the ionization balance of the plasma. The EBIT experiments were the first measurements of charge state distribution

of a heavy-element (gold) plasma in coronal equilibrium [*Physical Review Letters* **90**, 235001 (2003)]. In this regime, available models do not adequately reproduce the measured distributions, pointing out the need for further improvements in the theoretical models.

Robert Heeter (heeter1@llnl.gov) and
Mark May (may13@llnl.gov)

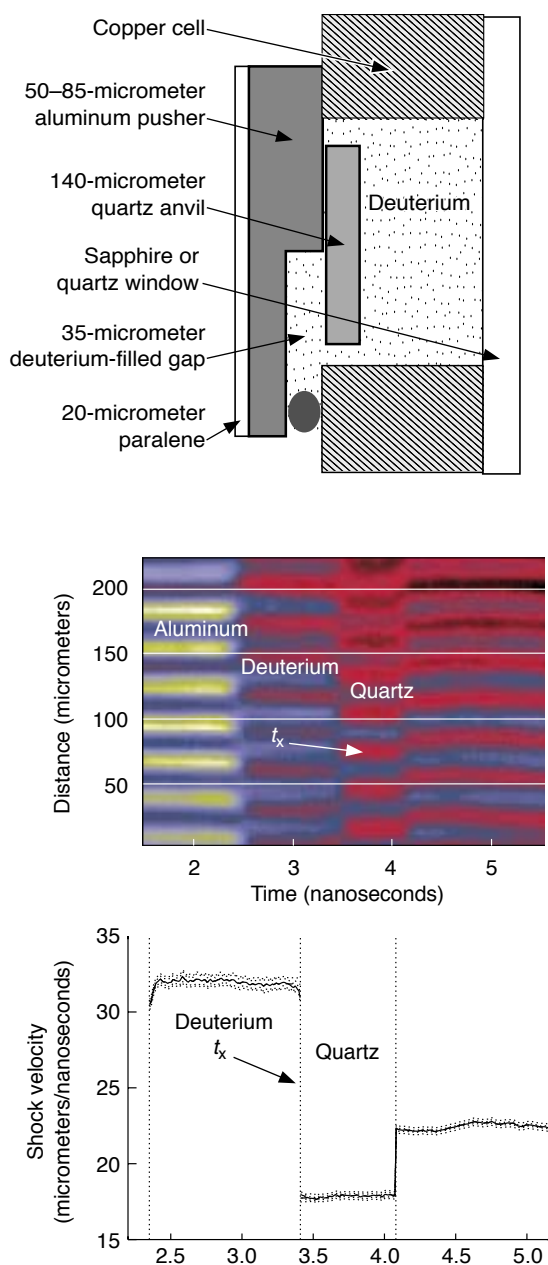
High-Pressure Equations of State of Heavy Elements

Livermore programs require accurate EOS of materials at pressures above 1 gigabar (Gbar). Yet, there are relatively few measurements at pressures greater than a few megabars (Mbar), and the existing data are significantly less precise than those obtained on gas guns at lower pressures. High-power lasers have the potential to generate shock pressures far in excess of those achievable on other currently available devices. For example, NIF is expected to produce shock strengths in the Gbar range using either x-ray or direct-laser illumination. Using these high pressures for precision measurements will require understanding and mitigating the deleterious effects of the high laser intensities needed to drive these high-pressure shocks. Establishing precise control of laser performance is also essential as is development of high-quality techniques for target fabrication and metrology.

To address some of these issues, we have conducted experiments on the Omega laser to study both shock steadiness and preheat of the target. Steadiness has been measured using high-Z targets with steps and VISAR measurements of shock propagation in transparent materials. The results show that the currently available four-beam NIF laser can be used to drive shocks in high-Z materials at pressures over 100 Mbar. Other experiments characterized potential preheat of the targets by fast electrons. The measured preheat levels indicate that preheating of the target will not be an issue for accurate EOS measurements at the laser intensities required for driving Gbar shocks on NIF.

During 2004, experiments will be conducted on the NIF laser to develop the capability for ultrahigh-pressure EOS measurements. The initial experiments will commission the VISAR diagnostic used for precise velocity measurements. These experiments will be followed by others to characterize the pressure drive delivered to targets and to measure the EOS of copper along

3 Schematic representation of the special target used to generate multiple shocks in a deuterium sample (**top**). Image of the interference fringes obtained with the VISAR diagnostics (**middle**). Analysis of the fringe shifts provides the velocity of the shock as a function of time (**bottom**). The first jump occurs at about 2.4 nanoseconds when the shock crosses the aluminum-deuterium interface; the second discontinuity occurs at about 3.4 nanoseconds (shown as t_x) when the shock velocity drops to a lower value as it enters the quartz window.



the principal Hugoniot to 23 Mbar. These first experiments will commission the NIF as a high-pressure EOS platform, providing a capability for EOS measurements at pressures previously available only in experiments driven by nuclear explosions.

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High-Pressure Equation of State of Hydrogen

Hydrogen is the most abundant element in the universe. It is the principal constituent of stars and of Jupiter, Saturn, and observed extra solar planets; the fuel of ICF targets; and integral to the Stockpile Stewardship Program. Understanding the high-pressure EOS for hydrogen is key to establishing accurate evolutionary and structural models for these planets and stars, a predictive capability for tuning ICF ignition capsules, and a complete understanding of weapons physics.

The principal Hugoniot of deuterium near 1 Mbar has been measured recently with two different techniques, one using a laser driver and one using a magnetic flyer. (The principal Hugoniot is often used to constrain EOS models at high pressures and temperatures because it can be measured and is well defined.) These two published measurements show significantly different compressibilities, and there is currently no scientific resolution to this discrepancy. In addition to the above mentioned measurements, there are double-shock experiments from the NIKE laser, a convergent single-shock measurement using a high-explosive driver, and a variety of gas-gun experiments. There is agreement between the convergent single-shock datum and the single-shock magnetic-flyer data. Both experiments use an impedance match technique with aluminum as the standard. There is also agreement between the Nova laser Hugoniot data [*Science* **281**, 1178 (1998)], the NIKE laser double-shock data, and gas-gun data within the framework of existing models. However, the discrepancy between the magnetic-flyer and laser-driven measurements is not resolved. The collection of all these results suggests that our current understanding of the EOS of compressed hydrogen is incomplete.

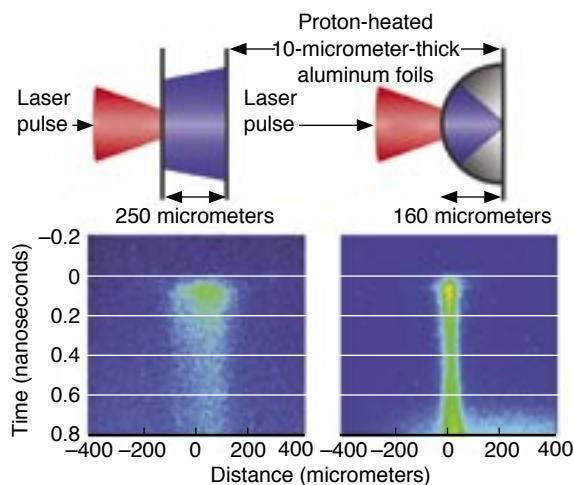
In collaboration with colleagues at the University of Rochester, we have conducted additional experiments to probe the compressibility of fluid deuterium up to several Mbar using laser-driven shock waves reflected from a quartz anvil (Figure 3). The

combination of high-precision shock-velocity measurements with the double-shock technique, where differences in EOS models are magnified, produces experimental data that are able to discriminate between various theoretical predictions. No current theory can adequately account for the observed double-shock results over the entire range of pressures investigated. Ab initio theoretical predictions are consistent with the measurements for first-shock pressures below 1 and above 2 Mbar, but disagree at intermediate pressures. Thus, the EOS of hydrogen at Mbar pressures and eV temperatures remains an open question to be resolved by further experimental and theoretical research.

Damien Hicks (hicks13@llnl.gov)

Energetic Proton Production in Ultrahigh-Intensity Laser Interactions

We are investigating the use of ultrahigh-intensity, short-pulse lasers to study the physical properties of high-temperature plasmas near solid density. In recent years, experiments at Livermore and elsewhere have demonstrated that the interaction of an ultraintense laser pulse with a solid target produces an intense, short-duration, and highly directional proton beam emitted from the rear surface of the target. This intense beam of protons is well suited for rapidly and uniformly heating samples to high temperatures at solid density—conditions where the physical properties of plasmas, such as EOS, are not well understood. The goal of our current research effort is to use one beam of protons to heat the sample and then use a second proton beam, delayed with respect to the first, to radiograph the heated sample and



4 Schematic representation of the flat and hemispherical targets heated with ultrashort laser pulses to generate proton beams (**top**). Streak camera images showing temporal and spatial dependence of the thermal emission from foils heated by the proton beams (**bottom**). These images are analyzed to infer the temperature profile of the proton-heated material. The hemispherical target produces a focused proton beam that heats the foil to higher temperatures.

measure the release wave. The sound speed can be measured with sufficient accuracy to distinguish between different EOS models currently used for the high-temperature, solid-density regime.

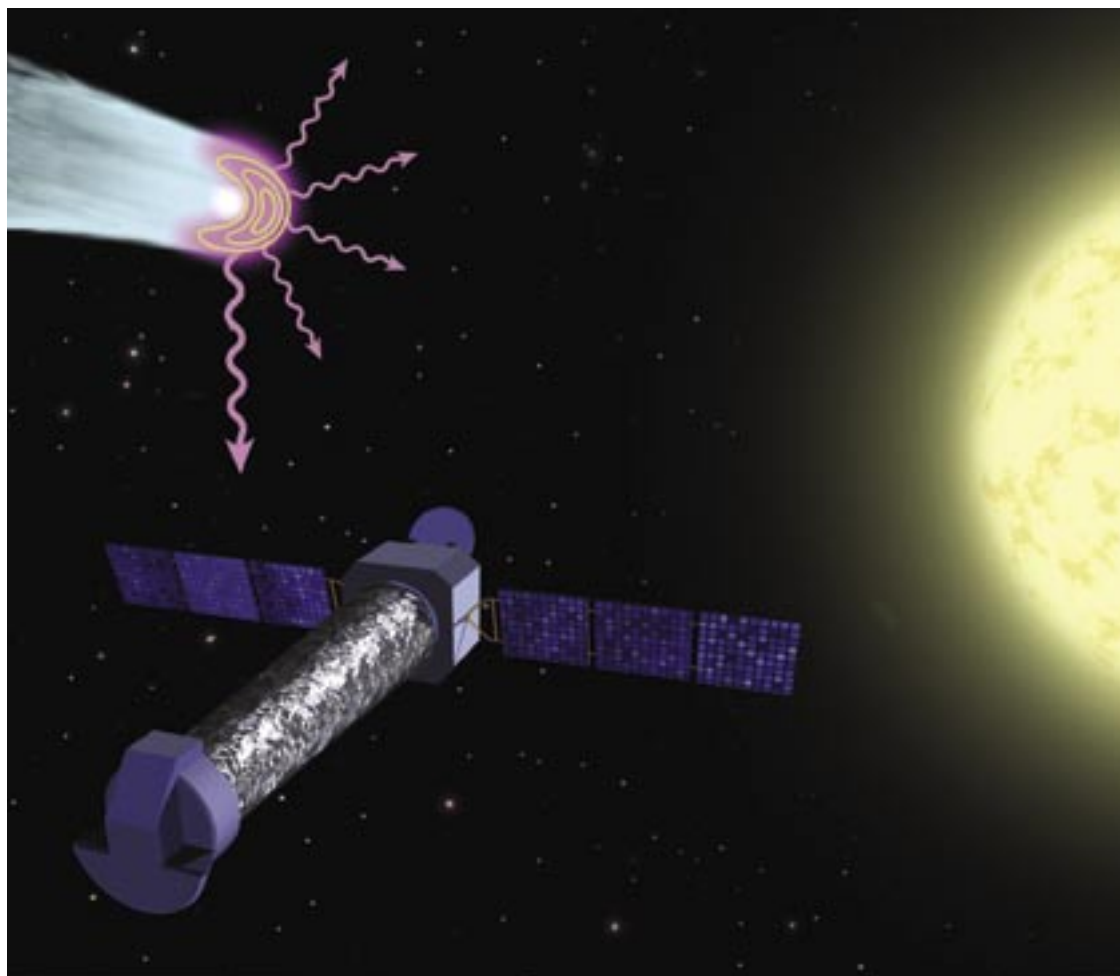
During 2003, a team led by a V Division scientist used the JanUSP laser to demonstrate isochoric (constant volume) heating of solid-density matter with an ultrafast proton beam (Figure 4). Using protons generated from flat targets, the team heated solid-density aluminum samples to 4 eV (roughly 50,000 kelvins). Spherically shaped targets produced a focused proton beam that heated samples to 23 eV [*Physical Review Letters* **91**, 125004 (2003)].

These results were highlighted in *Physical Review Focus* (September 22, 2003).

In the coming year, this technique will be combined with a second proton beam to obtain radiographic images and measure the release wave in high-temperature, solid-density plasmas. This capability, when fully developed, will enable researchers to perform measurements in regimes of importance to Laboratory programs where no good theoretical models exist and where there are few previous experimental data to guide theories.

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5 A continuous stream of charged heavy ions in the solar wind collides with gases surrounding the nucleus of a comet. The collision is thought to neutralize the solar wind ions and to induce them to give off x rays characteristic of the ions and gases involved in the collision (upper left). This process was successfully simulated at the Electron Beam Ion Trap using a detector from Goddard Space Flight Center to record the x-ray emission produced by charge exchange.



X-Ray Emission from Comets

X-ray satellite observations have firmly established comets as x-ray sources, a discovery that has far-reaching implications for understanding their interaction with the inner solar system. This discovery has opened up a new wavelength band for probing the solar wind—space weather—in real time, studying the interactions between comets and the sun, and understanding the composition of cometary atmospheres. Charge exchange between heavy ions in the solar wind and cometary gases is a leading candidate for the mechanism of x-ray production from comets (Figure 5). However, because the charge-exchange process is poorly understood for solar wind ions, models of charge-transfer-induced x-ray emission, based on best estimates, have not been able to reproduce the observed soft x-ray emission.

We completed a research project on EBIT that investigated the x-ray emission produced by charge exchange between neutral gas and highly charged carbon, nitrogen, and oxygen ions. The measured spectra did not match predictions from the theories used previously to estimate charge-exchange-induced x-ray production in comets. Based on results of the EBIT experiments, a new charge-exchange emission model was developed that successfully reproduced the soft x-ray spectrum of comet Linear C1999 S4, observed by the Chandra X-Ray Observatory. This work clearly demonstrated that an emission model based solely on charge-exchange processes involving solar wind ions can account for the

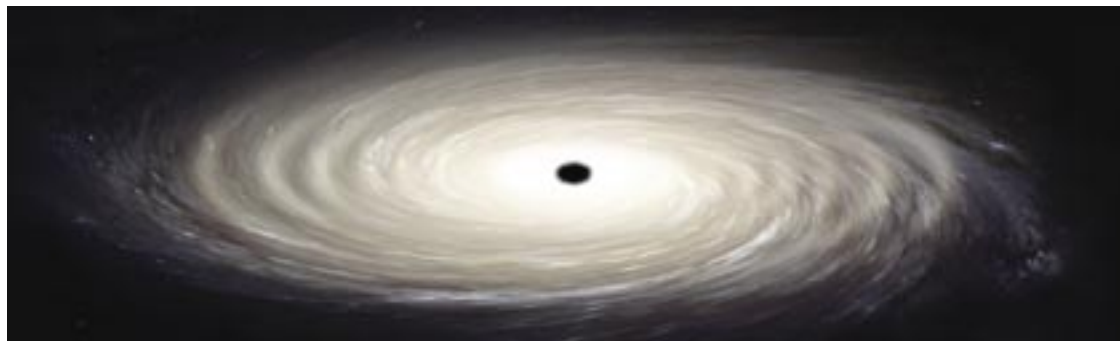
x-ray spectra observed from comets [*Science* **300**, 1558 (2003)].

Peter Beiersdorfer (beiersdorfer1@llnl.gov)

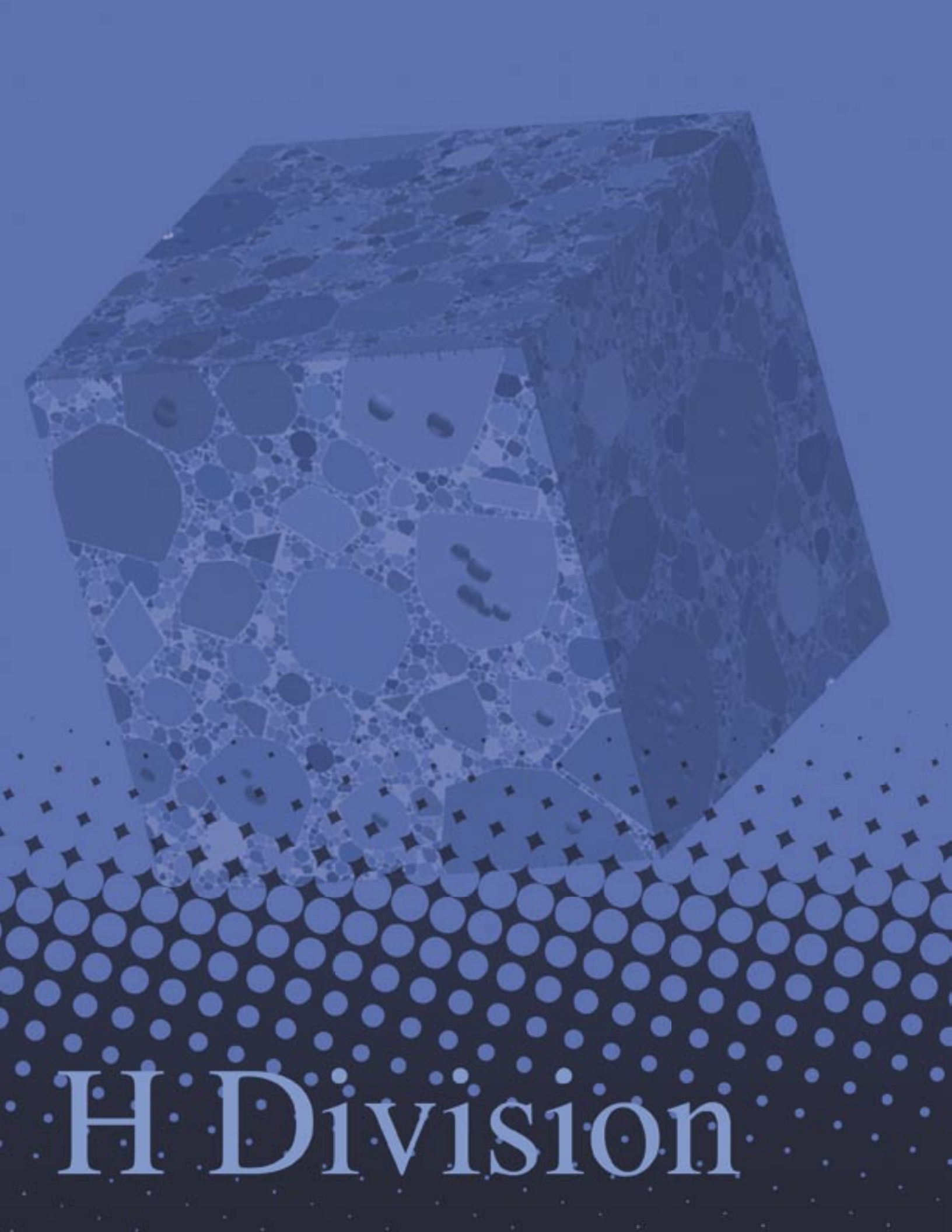
X-Ray Production from Black Hole Accretion Disks

Recently, the Chandra and XMM-Newton x-ray satellite missions have observed broad spectral features in the soft x-ray spectra of type-1 Seyfert galaxies. A controversial interpretation is that these features are relativistically broadened and gravitationally red-shifted emission lines that arise from an accretion disk in the extreme gravitational field around a black hole. The controversy persists because the simple models used to compute the spectra that would be observed from such an object apparently do not contain all the fundamental physical effects present. With collaborators from Massachusetts Institute of Technology and Harvard-Smithsonian Center for Astrophysics, we have constructed a new computational model that combines detailed atomic spectral data with an accretion disk atmosphere model and uses a Monte Carlo treatment of radiation transfer. This more complete and detailed model can describe the considerable reprocessing of the soft x-ray radiation produced near the black hole as it propagates through the rest of the accretion disk (Figure 6). Currently, the team is incorporating additional relativistic physics that affects the propagation of the radiation in the gravitational field of the black hole. The new model will allow detailed comparisons of the computed soft x-ray spectra with the observations.

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6 Artist's rendering of a black hole surrounded by the accretion disk, which consists of material drawn toward the black hole by its gravitational field. The region near the black hole emits x rays. As the x rays travel through the accretion disk toward the observer, the spectrum of the x rays is altered.



H Division

CONDENSED MATTER PHYSICS DIVISION

The Condensed Matter Physics Division (historically known as H Division) emphasizes research on the properties and behavior of matter under extremely high pressures and temperatures. H Division combines unique experimental and theoretical capabilities with Laboratory resources to create a world-class center for research in condensed matter physics and materials science. A major goal is to advance the fundamental condensed matter science that underpins Laboratory programs in stockpile stewardship, defense, energy, and nonproliferation.

We possess internationally recognized expertise and engage in active research in a number of areas. The experimental program includes such activities as:

- High-pressure and high-temperature measurements using diamond-anvil cells and other techniques.
- Development and use of x-ray techniques at synchrotron light sources for investigating material properties.
- Precise high-pressure measurements of material dynamics using light-gas guns.
- Shock production and short-timescale measurements using energetic lasers.

The theory and modeling program includes such activities as:

- Fundamental and algorithmic development of first-principles quantum methods.
- Development and application of advanced numerical methods for simulating material properties and behavior.
- Simulation and modeling of dynamic processes in condensed matter.
- Advanced statistical mechanics applied to materials at extreme conditions.

Current emphasis encompasses the following research areas:

- Actinide science and physics of metals at high pressure and temperature.
- Descriptions of matter at high-pressure, finite-temperature conditions attained in experiments at the National Ignition Facility and other lasers, and those relevant to

geophysics, astrophysics, and other extreme phenomena.

- Dynamics and kinetics of high-pressure matter.
- Computational description of the properties of organic and inorganic nanometer-sized particles.
- Synthesis and experimental characterization of nanoparticles.
- High-explosive materials and detonation physics.

Our research program makes use of a number of special facilities:

- An advanced high-pressure laboratory with diamond-anvil and other high-pressure cells, thermal and laser heating equipment, and multiple diagnostics.
- Two fully instrumented light-gas guns capable of 8-kilometer-per-second projectile speeds.
- A nanoparticle synthesis and characterization laboratory.
- Supercomputers sponsored by the Advanced Simulation and Computing (ASC) Program.
- Beamlines at several synchrotrons, including a partnership with the High Pressure–Collaborative Access Team (HP-CAT) beamline at the Advanced Photon Source at Argonne National Laboratory.
- The Joint Actinide Shock Physics Experimental Research (JASPER) facility at the Nevada Test Site.

H-Division scientists collaborate extensively with researchers from other Laboratory organizations as well as the general scientific community. During 2003, they partnered and published with colleagues from more than 70 academic institutions in 17 countries.

Shock Physics Experiments

Shock physics experiments provide accurate information about the equation of state (EOS) of materials at high pressures. Motivated by the need for such data for actinides, the Stockpile Stewardship Program has constructed JASPER at

the Nevada Test Site. JASPER uses a two-stage light-gas gun to launch projectiles at plutonium targets to generate high dynamic pressures. After a 20-shot series to test the gun, diagnostic equipment, and containment systems, JASPER was first used for plutonium EOS experiments during the summer of 2003. To date, we have performed four experiments with JASPER on delta-phase plutonium with unprecedented accuracy and precision. The measurements are unique in that we obtained absolute determinations of pressure, density, and internal energy up to pressures of about 6 megabar. These initial experiments are the first phase of a decade-long program to determine the EOS, phase boundaries, and constitutive properties of plutonium.

While the initial JASPER experiments all used simple shock loading, we have developed recently a novel pressure-loading method, which

uses impactors with a designed density profile to produce a wide range of stress-versus-time profiles. Using these new impactors in gas-gun experiments will enable researchers to produce a much wider range of physical conditions, thus greatly expanding the utility of JASPER for basic plutonium science and programmatic applications.

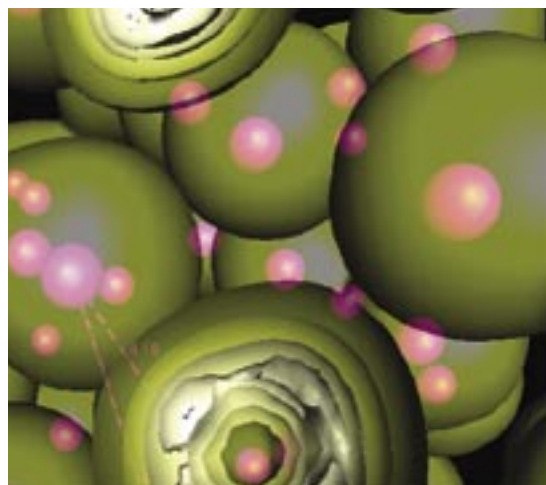
The science of phase-transition kinetics at high shock pressures is growing in interest and importance. One recent example is the new melting point for iron at Earth's inner-core conditions [*Nature* **427**, 339 (2004)]. In this work, we used sound-velocity measurements to determine the loss of shear strength, indicating that melting has occurred. On the other hand, we found no evidence for a putative solid–solid phase transition in iron that bedeviled theorists for two decades. An important lesson learned from these experiments was the need for new methods to determine not only the phase boundaries, but also the timescale of phase transition. Currently, we are investigating new optical techniques that may fulfill this need. We plan to apply the recently demonstrated methods to the study of melting and resolidification of metals under quasi-isentropic loading.

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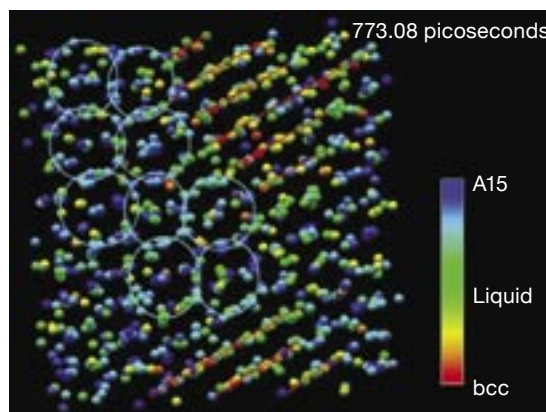
Quantum Simulations of Actinide Metals

The development of highly accurate multiphase EOS for actinide metals requires a fundamental theoretical understanding of their properties at the quantum-mechanical level. Quantum molecular dynamics (QMD) is an advanced simulation that allows one to treat the motions of electrons and ions on an equal footing, so that the thermodynamic and structural properties of both the high-temperature solid and the liquid can be investigated from first principles. For actinide metals, however, QMD simulations are extremely challenging because of the number of electrons that must be considered (14 per atom for uranium and 16 for plutonium), the complexity of the electronic structure, and the slow motion of the heavy ions relative to the simulation time. In 2003, we developed new, efficient QMD algorithms for high-opacity (high-*Z*) metals, and with the aid of the ASC supercomputer Q at Los Alamos National Laboratory, we performed the first-ever quantum simulations of an actinide metal, uranium (Figure 1). These simulations, which are being continued on the ASC White machine at Livermore, will play an important role

1 Snapshot from a quantum molecular dynamics simulation of liquid uranium at a temperature of 2275 kelvins and a pressure of 15 kilobars. The simulation was performed on the Advanced Simulation and Computing supercomputer Q at Los Alamos National Laboratory. Here, the green “onion skins” represent electron-density contours, and the pink balls represent ion positions within the computational cell.



2 Snapshot from a large-scale molecular dynamics simulation of rapid resolidification in tantalum. The colored balls represent the positions of individual atoms. The blue circles indicate regions of a nucleating A15 structure, while the red solid lines identify regions of tantalum recrystallizing into the body-centered cubic (bcc) structure.



in helping researchers develop the next-generation multiphase EOS for plutonium.

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Atomistic Simulation of Rapid Resolidification

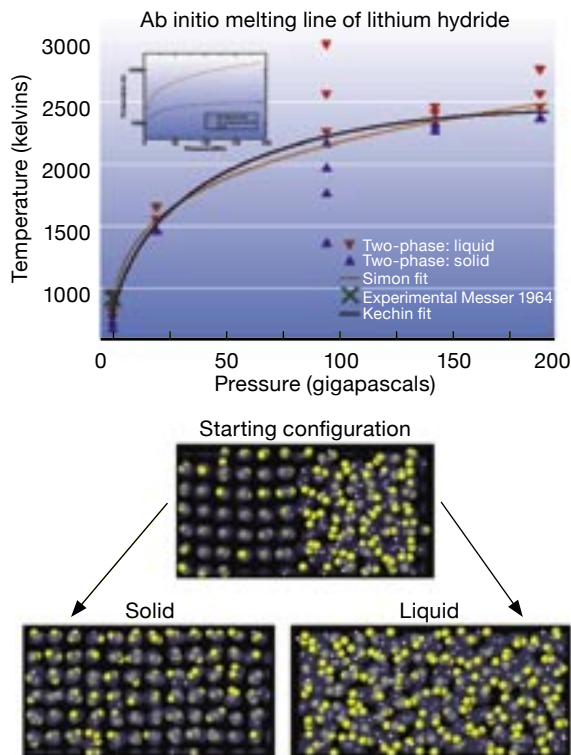
Although the kinetics of phase transitions is a potentially important aspect of multiphase EOS, strength, and failure, it has received little attention. To address this issue, H Division has undertaken a coordinated research program involving both theory and experiment. Our initial focus has been on the rapid resolidification of metals, whereby, for example, an initially molten metal is rapidly compressed across the high-pressure melting curve. Here the goal is to understand both the atomic and microstructural morphology of the final resolidified phase, together with the timescales on which this morphology was developed. We are using quantum-based many-body interatomic potentials in large-scale molecular dynamics simulations to investigate the nucleation and early growth of the resolidified phase. In 2003, we performed revealing simulations on tantalum that give clear evidence of a metastable, low-symmetry A15 phase in the solidifying melt, which slows—by two orders of magnitude—the kinetics of recrystallization into the body-centered cubic form (Figure 2). Similar calculations are also being performed on other metals such as bismuth, for which complementary gas-gun experiments using new graded density impactors are currently under way (see the Shock Physics Experiments section).

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First-Principles Calculations of Melting Temperatures

Accurate first-principles computational methods provide a detailed description of structural and bonding changes in a material as it undergoes phase transition at extreme conditions. An example is melting temperature as a function of pressure. However, given the high computational cost in determining phase boundaries, first-principles simulations have been used in only a few cases to compute melting temperatures. Specifically, calculations of the free energies employing the so-called potential switching method (which relies on the existence and accuracy of an empirical reference potential) were used to determine the melting temperatures of silicon, aluminum, and iron at high pressures.

To overcome the need for empirical reference potentials and thus design a fully ab initio tool, we



3 Melting line of lithium hydride as determined by first-principles simulations (**top**) compared to simple models (see inset, where a comparison with Livermore equation-of-state data is given). A ball-and-stick representation of atoms in the two-phase simulation (**bottom**).

carried out calculations of melting temperatures by directly comparing the free energies of solid and liquid phases using a so-called two-phase simulation method (Figure 3, bottom).

We have applied this new, fully ab initio technique to the calculation of the melting temperature of lithium hydride (LiH) as a function of pressure [*Physical Review Letters* **91**, 175502 (2003)]. The predicted melting temperature (Figure 3, top) varies slowly with compression at high pressures, ranging from 2000 to 2450 kelvins (K) in the 50- to 200-gigapascal (GPa) pressure range. These temperatures are very different from those derived from simple models (Figure 3, inset). In addition, we have investigated the structural and bonding properties of the molten state of LiH. Results show that, close to the melt line, the compressed fluid retains the ionic character of the low-pressure molten state. At higher temperatures, we observed dynamic hydrogen clustering processes, which are accompanied by significant changes in the electronic structure of the liquid.

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Simulation of Grain-Scale Dynamics of Explosives

Changes in the microscopic properties of an explosive can affect its performance. For example, it has long been recognized that the sensitivity of most explosives is dramatically affected by voids (typically 10 micrometers) within individual molecular crystals (typically 100 micrometers) or between them (Figure 4). To use explosives as an engineered material requires control of this sensitivity. Too little sensitivity and the explosive will not detonate when desired. Too much sensitivity and the explosive assembly becomes too dangerous to handle.

We are using computational models to simulate the response of explosives to external mechanical stimuli at the grain-scale level. The ultimate goal is to understand in detail the complex processes associated with the material response, so scientists can develop realistic material models for use in multiphysics hydrodynamics codes. Such codes are widely used at the Laboratory to model real systems. The present research focus is to use the results of grain-scale simulations to develop an advanced macroscopic reactive flow model that is consistent with our understanding of the grain-scale details and incorporates such information quantitatively. The objective is to correlate changes in the observed properties of the explosive (e.g., grain size distribution; binder thickness distribution; void shape, size, and separation distribution; binder mechanical properties) with predictions of the explosive's sensitivity and performance.

In 2003, we used supercomputers and software developed under the ASC Program to examine

the detailed behavior of explosive assemblies with voids when they are exposed to shock waves. We carried out quantum molecular dynamics simulations to check the models of chemical reaction rates at high pressure and temperature (typical values are 30 GPa and 3000 K). Classical molecular dynamics simulations were used to test models of the EOS and transport properties of the gaseous decomposition products over a range of pressure and temperature (0.0001 to 100 GPa, 300 to 30,000 K). We also used elastic-plastic hydrodynamics simulations that couple chemical reaction rates and heat transfer to evaluate initiation and growth of the reaction in explosive assemblies.

John Reaugh (reaugh1@llnl.gov)

Discovery of "Bucky Diamond"

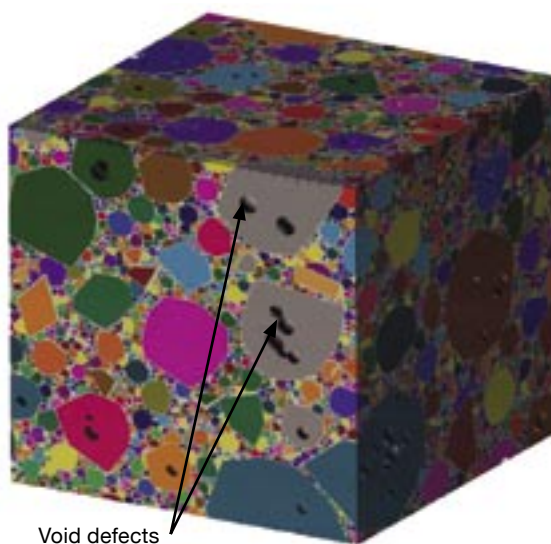
Nanometer- (nm-) sized diamond (a form of carbon) has been found in meteorites and interstellar dusts as well as in residues of detonation and in diamond films. Remarkably, the size distribution of diamond nanoparticles appears to peak around 2 to 5 nm and is largely independent of the conditions under which they are formed.

In 2003, we carried out first-principles, quantum mechanical calculations to investigate the structure of such carbon nanoparticles [*Physical Review Letters* **90**, 037401 (2003)]. Results show that in the 2- to 5-nm range, the nanoparticles have a diamond core and a fullerene-like surface and, unlike silicon and germanium, exhibit very weak quantum confinement effects. In a reference to the famous buckyball form of carbon, we named the nanoparticles with a diamond core and a fullerene-like surface, "bucky diamond" (Figure 5).

Furthermore, first-principles calculations were performed to study the stability of nano-diamond as a function of surface hydrogen coverage and size [*Nature Materials* **2**, 792 (2003)]. We found that at about 3 nm and for a broad range of pressure and temperature, particles with bare, reconstructed surfaces become thermodynamically more stable than those with hydrogenated surfaces, thus preventing formation of larger grains. These results provide an explanation of the size distribution of extraterrestrial and terrestrial nanodiamond found in ultradispersed diamond films. They also offer an atomistic structural model of these films, based on the topology and structure of 2- to 3-nm-sized bucky diamonds.

Guilia Galli (galligygi1@llnl.gov)

4 Simulation of void defects. The cube shown here contains 100,000 crystals of explosive with 2 volume percent of internal defects represented as spherical voids. Those that intercept the faces of the cube can be seen as divots in the plane faces.



High-Pressure Experiments at a Dedicated High-Pressure X-Ray Beamline

In collaboration with Carnegie Institute of Washington and University of Nevada at Las Vegas, H Division scientists have developed a dedicated x-ray beamline named the High Pressure–Collaborative Action Team (HP-CAT) beamline at the nation's brightest third-generation synchrotron, the Advanced Photon Source at Argonne National Laboratory. The Department of Energy-sponsored HP-CAT beamline provides a new, state-of-the-art capability for experimental investigations of the high-pressure properties of materials, including those relevant to the Stockpile Stewardship Program. Construction was completed in June 2003, and the beamline commissioned for experiments shortly thereafter. Examples of cutting-edge materials-science experiments under way include inelastic x-ray scattering to explore electronic structure and lattice phonons and to determine the structure of high-density liquids, and single-crystal diffraction applied to small single-crystal grains (less than 0.01 millimeter) contained within polycrystalline samples in diamond-anvil cells.

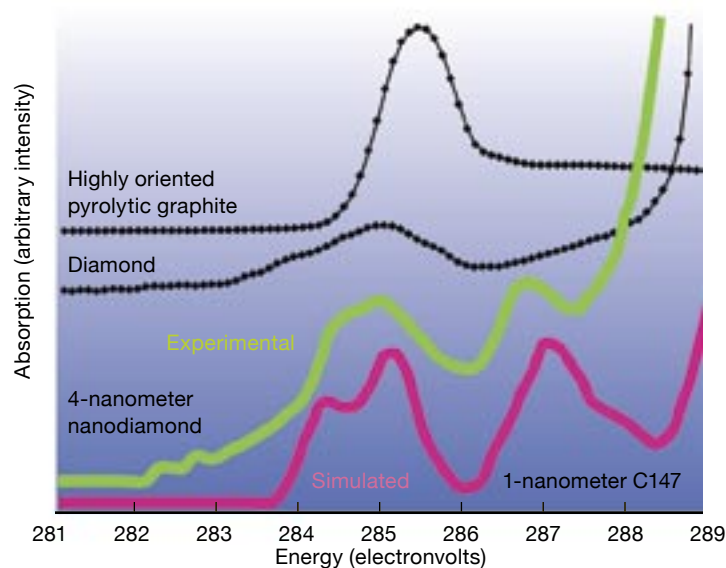
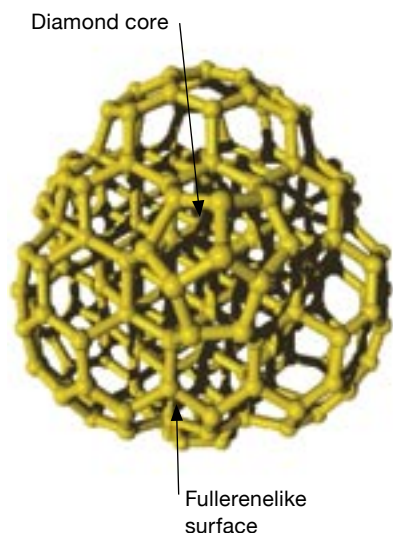
Accurately determining crystal, electronic, and phonon structures of dense fluids and solids at high pressures and temperatures has long been a formidable experimental challenge, even for simple elements. Not only is it difficult to create these extreme conditions in the laboratory, the diagnostic techniques available were not suitable for

the minute samples that can be produced at those conditions. With recent developments of diamond-anvil cell technologies, coupled with x-ray microprobe-based diagnostic methods available at the HP-CAT beamline (Figure 6), we made significant progress in unraveling the high-pressure properties of stockpile materials, including plutonium. Even though plutonium possesses the most complicated phase diagram of all elements, with many ill-characterized polymorphs, in 2003 we succeeded in characterizing the crystal structure of a high-pressure phase settling a long-standing controversy. The experiments also led to the discovery of a new phase and provided phase-specific data critical to the ongoing theoretical development of the next-generation multiphase EOS and strength models for the nation's Stockpile Stewardship Program.

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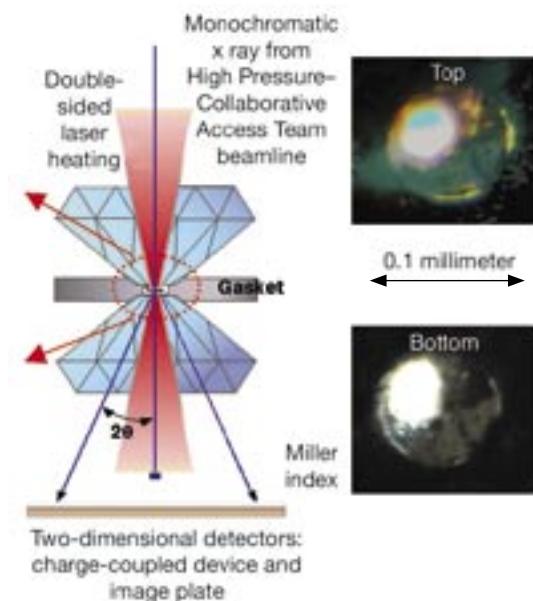
Discovery of Super-Hard Polymeric Carbon Dioxide

Recently, we discovered that dramatic changes occur in the molecular configuration, chemical bonding, intermolecular interaction, and crystal structure of carbon dioxide (CO_2) at high pressures and temperatures. Previously, CO_2 had commonly been considered a stable solid consisting of linear molecules. New phases include a tetrahedrally bonded CO_2 polymer similar to silica- (SiO_2 -) quartz, a phase consisting of bent CO_2 molecules

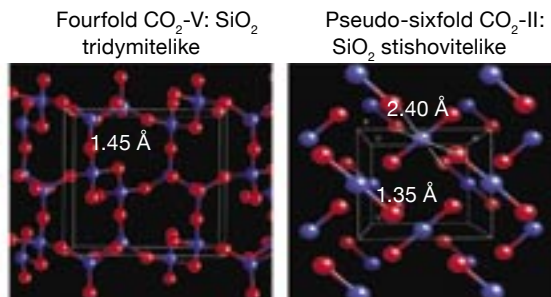


5 Ball-and-stick representation of bucky diamond (left), whose structure was determined by first-principles simulations and confirmed by spectroscopic measurements carried out by Livermore scientists at the Advanced Light Source at Lawrence Berkeley National Laboratory (right).

6 In situ high-pressure and high-temperature x-ray diffraction experiment with a plutonium sample contained in a double-sided, laser-heated diamond-anvil cell (**left**). Images show the sample is being heated from both top and bottom (**right**).



7 Ball-and-stick models of the novel extended phases of carbon dioxide formed at high pressures and temperatures. These solids exhibit extremely low compressibility and optically nonlinear behavior with high conversion efficiency. (Å = angstrom.)



8 Transmission electron microscope image of germanium nanoparticles obtained by a new synthesis route. The particles, which are stable in air, have a diamond structure, as revealed by x-ray diffraction measurements.



an optically nonlinear crystal that converts infrared light into green light with a high conversion efficiency. It also has an extremely low compressibility (bulk modulus of 361 GPa, which is comparable to that of cubic-boron nitride at 362 GPa) and thus is likely to be super hard. It is also metastable to pressures far below its formation pressure, providing opportunities to engineer new materials with unusual optical, mechanical, and energetic properties. While the results obtained for CO₂ demonstrate proof of principle for producing exotic metastable phases by application of high pressures, similar transitions to extended phases are expected in many other molecular solids.

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Theoretical and Experimental Investigations of Semiconductor Nanoparticles

Close interaction of experimental and theoretical research on semiconductor nanoparticles is essential to the design, synthesis, and characterization of such materials that have predetermined mechanical, electronic, and optical properties. A closely coordinated effort in H Division made significant progress in this area in 2003.

On the experimental side, a team led by H Division researchers developed a novel two-step synthesis route, which yielded grams of nanometer-sized germanium crystals in the form of a black powder [*Nano Letters* (March 13, 2004)]. The presence of pure germanium is illustrated by x-ray diffraction measurements and transmission electron microscope images (Figure 8). The as-synthesized powders are stable in air for months, and no oxidation occurs. The results of these experiments call for caution in interpreting the high-pressure, high-temperature synthesis of silicon and germanium nanoparticles reported in the recent literature.

While experiments have been successful in producing gram quantities of germanium nanoparticles and encouraging results have been obtained for silicon as well, a full experimental characterization of the surface properties of these clusters is difficult to obtain. First-principles, quantum mechanical calculations are an ideal

way to study the atomic surfaces of silicon nanoparticles with different hydrogen content and reconstructions [*Physical Review Letters* **91**, 157405 (2003)] and to investigate the attachment of small organic molecules to silicon clusters (Figure 9).

Guilia Galli (galligygi1@llnl.gov)

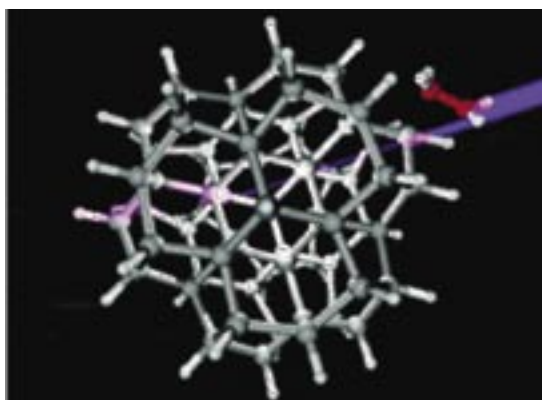
New Class of High-Energy-Density Materials

Extended solids of covalently bonded light elements constitute a new class of high-energy-density materials (HEDM) with dramatically enhanced performance and great potential for defense applications. Previously, we demonstrated the existence of this class of HEDM by synthesizing solid polymeric carbon monoxide, cyanide, and nitrogen at high pressures in diamond-anvil cells. Our calculations predict that such extended solids could have dramatically enhanced energy densities of about three times that of HMX, a commonly used high explosive.

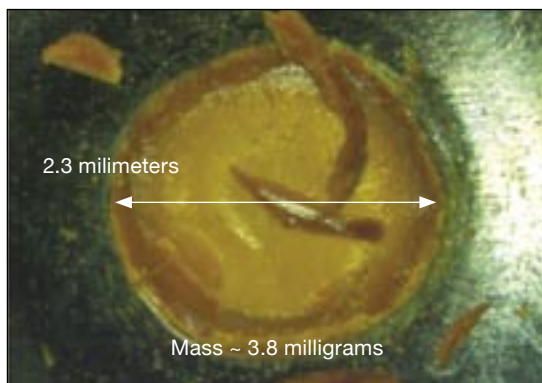
Detailed characterization of the structure and energetics of these HEDM has been a challenge because of the minute amount of the sample and its high metastability. Therefore, we put a significant effort into the synthesis of a larger, milligram quantity of carbon monoxide polymers using a large-volume, high-pressure Paris-Edinburgh cell (PEC). In 2003, we successfully demonstrated, for the first time, that we can load a toxic, cryogenic fluid into the PEC and produce a substantial quantity (typically 1 to 10 milligrams) of the carbon monoxide polymer (Figure 10).

With successful synthesis of relatively large samples, we are now investigating the three issues that are critical to potential applications of this HEDM: energetics, structure, and metastability. We are using a wide range of analytical tools, such as a differential scanning calorimeter, carbon-13 magic angle spinning nuclear magnetic resonance, and shock impulse measurements to characterize the sample. The goal is to elucidate the relationships among the chemical structure, energetics, and metastability of solid polymeric carbon monoxide and thus optimize synthetic conditions and enhance HEDM performance.

Choong-shik Yoo (yoo1@llnl.gov)



9 Ball-and-stick representation of the attachment of a hydrocarbon group to a silicon cluster. Ab initio calculations show that the probability of attachment is greatly increased when the cluster is in an excited state prior to the chemical reaction [*Journal of the American Chemical Society* **125**, 15243 (2003)].



10 Large sample of a solid polymeric carbon monoxide synthesized at 5.8-gigapascal pressure using a large volume press of the Paris-Edinburgh type.



N Division

NUCLEAR, PARTICLE, AND ACCELERATOR PHYSICS DIVISION

The Nuclear, Particle, and Accelerator Physics Division (known as N Division) leads the Laboratory in experimental and theoretical nuclear physics and experimental high-energy physics. Activities include research and development of relevant accelerator and detector technologies, nuclear databases, nuclear-physics-intensive computer simulations, and experiments on nuclei and elementary particles.

In support of the Stockpile Stewardship Program, N Division plays a major role in the Physical Data Research Program. Our primary responsibility is to provide fundamentally derived and fully evaluated nuclear data (such as fission and fusion reaction rates) required for computational simulation of nuclear-weapons performance and tests. Such data are obtained from a combination of state-of-the-art measurements, first-principles-based theoretical calculations, and models validated against available experimental data.

In the area of nuclear physics, we have a strong and coordinated research effort in theory, modeling, and experiments. Current areas of emphasis include measurements of neutron-induced reaction rates, gamma-ray spectroscopy, measurement of radiochemical data required for analyzing past underground tests of nuclear weapons, development of advanced models for nuclear structure and fission, and determinations of nuclear spallation yields.

We are also responsible for developing and maintaining certain nuclear-physics-intensive simulation codes and software. These include three-dimensional Monte Carlo codes for modeling the transport of ionizing radiation through matter and the development of advanced computational techniques and algorithms suitable for Monte Carlo codes.

We conduct research on particle accelerator and detector technologies that are critical to the design and development of new experimental facilities. One example is technology enabling advanced radiography in hydrodynamic tests

conducted by the Stockpile Stewardship Program. In addition, we are a key partner in collaborative research programs in accelerator science and technology and high-energy particle physics sponsored by the Department of Energy (DOE) Office of Science. These research programs are centered at the Stanford Linear Accelerator Center in California, the Relativistic Heavy Ion Collider at Brookhaven National Laboratory in New York, and the Fermi National Accelerator Laboratory in Illinois. The work and accomplishments of N Division are helping to establish Lawrence Livermore as a center of excellence for accelerator science and technology and high-energy physics.

Measurement of Critical Nuclear Cross Section

A major goal for the Physical Data Research Program has been a precise measurement (within 10%) of the plutonium-239(n,2n)/plutonium-238 cross section. This cross section is particularly important because production of plutonium-238 by neutrons is a major diagnostic for interpreting underground nuclear tests.

Previous measurements of the cross section involved counting neutrons emerging from the interaction. This method was extremely difficult and subject to very large backgrounds. Results of several separate experiments and expectations based on nuclear modeling differed by large factors. Neutrons from other reaction channels—such as (n,n'), (n,3n), and (n,f)—form a background to the (n,2n) signal channel that makes a precise measurement difficult. Up to now, the lack of precise knowledge of the small plutonium-239(n,2n)/plutonium-238 cross section compromised the effectiveness of this important nuclear-test diagnostic.

Using its expertise in gamma-ray spectroscopy, the Nuclear Experiments and Technology Group in N Division invented a new approach to attack this problem [*Physical Review C* **65**, 021601 (2002)]. The experimental campaign took five years, involved collaboration with Los Alamos National Laboratory, and required construction of

a state-of-the-art detector array and extremely difficult analyses (Figure 1). This effort produced important experimental results for the yield of gamma rays as a function of neutron energy. Extracting the plutonium-239(n,2n)/plutonium-238 cross section from these results required an intensive and coordinated effort by the Nuclear Theory and the Computational Nuclear Physics groups of N Division. The final results are available to the nuclear weapon designers at both Lawrence Livermore and Los Alamos national laboratories, and have led to a critical reexamination of archived nuclear test data.

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Calculation of Nuclear Structure

The Nuclear Theory Group has embarked on a study to calculate from first principles the structure of nuclei—that is, how nuclei are put together. This is a fundamentally interesting physics problem because it involves the complex application of many-body physics to a system with strongly interacting constituents.

Understanding the structure of nuclei is important for several reasons. Nuclei are a key “laboratory” for testing the fundamental symmetries of nature. Nuclear structure strongly affects the rates of reactions that determine the course of stellar evolution and abundance of

elements in the universe. An improved understanding of nuclei also has many important applications to the national security mission of the Laboratory.

Performing these first-principles calculations of nuclear structure requires theoretical ideas from the nuclear shell model and effective interaction theory, along with the exceptional power of the massively parallel computers at the Laboratory, which are sponsored by the Advanced Simulation and Computing Program. Initial results for light nuclei showed that the calculation using our approach did converge on a solution. A serious disagreement between our calculated and the experimentally measured spectrum of boron (^{10}B) indicated, for the first time, that using only the two-body nucleon–nucleon interaction in the calculations does not lead to an accurate description of the nuclear structure. Our work provided compelling evidence that inclusion of three-nucleon interactions is critical in accurately determining the low-lying (low-energy) nuclear levels [*Physical Review Letters* **88**, 152502 (2002)].

The techniques used in our calculations have several advantages over other methods: they can treat general forms of the nucleon–nucleon force, provide a more extensive picture of the excitation spectrum, and are easier to extend to heavier nuclei. Information gleaned from this work also will help provide answers to questions regarding specific nuclear structure and reactions, such as $(n,n'\gamma)$, which are of interest to the stockpile stewardship and nonproliferation programs at Lawrence Livermore.

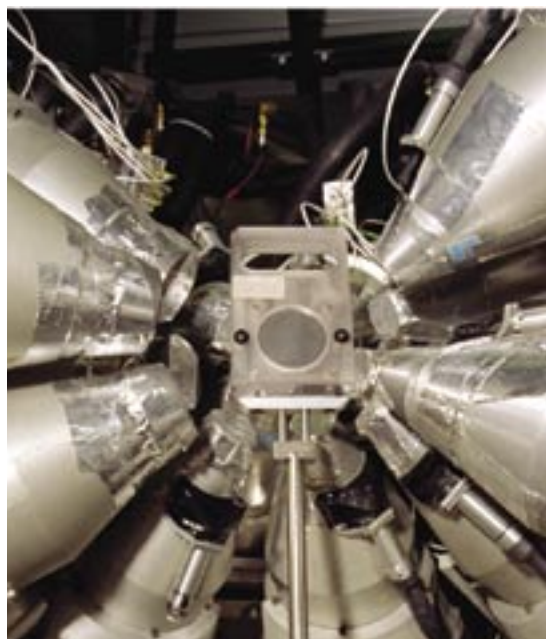
Erich Ormand (ormand1@llnl.gov)

Radioactive Ion-Beam Research

We continue to be involved in the emerging field of radioactive ion-beam physics. This research focuses on creating radioactive isotopes of elements and then accelerating them to high speed to study the nature of their interactions with fundamental particles and other nuclei. Many nuclear reactions important for our understanding of data from past underground nuclear tests involved radioactive nuclei.

We have been working at Lawrence Berkeley National Laboratory on the 88-inch cyclotron to develop innovative methods for producing usable beams of radioactive krypton. We used these

1 The detector known as Germanium Array for Neutron-Induced Excitations used to measure gamma rays emitted in neutron-induced nuclear reactions at the Los Alamos Neutron Science Center in New Mexico. The original version of this detector (the High Energy Resolution Array), used in experiments at Lawrence Berkeley National Laboratory, was moved to Los Alamos and upgraded in 1996. This detector played a central role in the five-year-long experimental campaign that led to an accurate determination of the cross section for the plutonium-239(n,2n)/plutonium-238 reaction—an important diagnostic for interpreting underground nuclear tests.



beams to study magnetic properties of particular isotopes as well as the possibility of measuring neutron reaction cross sections using an inverse kinematics approach. We also conducted experiments at Yale University and TRIUMF, Canada's national laboratory for particle and nuclear physics, that required the creation and manipulation of radioactive ion beams.

We actively participate in a large collaborative effort to formulate detailed plans for the Rare Isotope Accelerator Project sponsored by the DOE Office of Science. This project will develop the premier radioactive ion-beam facility in the world, which, after construction is completed, will enable the next generation of low-energy nuclear physics experiments. The roughly \$1 billion facility is currently in the design phase.

Lee Bernstein (bernstein2@llnl.gov)

Developing Radiographic Probes

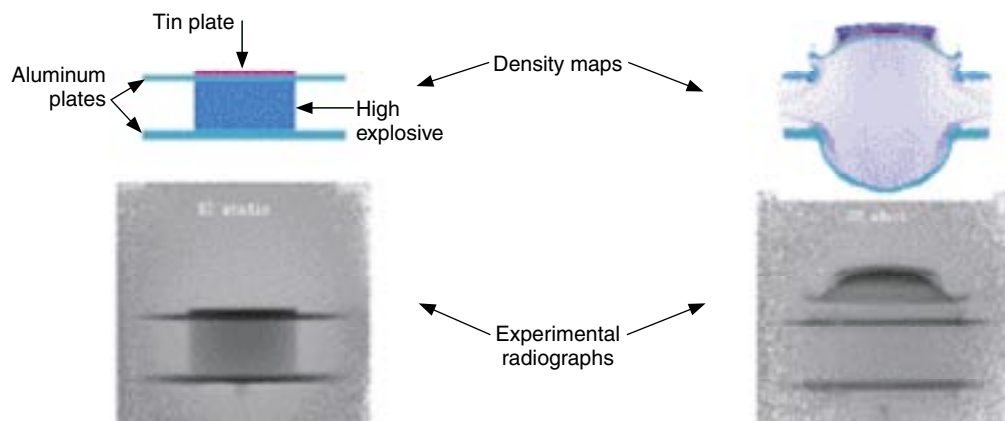
An advanced hydrodynamics facility (AHF), under consideration by the Stockpile Stewardship Program, would provide new experimental capabilities for studying the hydrodynamic behavior of stockpile materials and test assemblies. Use of very-high-energy protons is one candidate for the radiographic probe at the AHF, and we collaborated with colleagues at other national laboratories, including Los Alamos, to investigate this technique. We conducted experiments at the existing accelerator at Brookhaven National Laboratory in New York and are preparing for experiments at Fermi National Accelerator Laboratory in Illinois to measure fundamental particle-production cross sections relevant to the AHF [*Journal of Nuclear Science and Technology*, Suppl. 2, 1, 269 (2002)].

We also investigated the technique's ability to resolve small features and to measure the densities of material traversed by the high-energy protons. The results of these crucial measurements will help determine design parameters of the planned AHF.

In addition, we have made major contributions to a Livermore project to obtain quantitative measurements of the dynamic behavior of various materials under shock using high-energy protons as radiographic probes. These experiments have provided time-dependent pictures of metals and metal interfaces subjected to high-explosives-driven shocks (Figure 2). The experiments have permitted quantitative measurements of the shock velocity in the material and of the particles ejected from the surface. The precision of measurements has allowed detailed comparisons with hydrodynamics codes used at Lawrence Livermore. Future experiments will explore how metals tear or fracture under shock.

N Division leads the Laboratory's program to develop use of low-energy (10-megaelectronvolt) neutrons for radiography and tomography of static objects. Detailed three-dimensional simulations have shown that this technique can detect cubic-millimeter-sized defects in heavily shielded materials. The goal is to demonstrate the capability in proof-of-principle experiments at Livermore. Then it can be deployed at other DOE facilities, such as Pantex in Texas and the Y-12 facility in Tennessee, so that nondestructive evaluations of weapons components and assemblies can be made as part of the Enhanced Surveillance Program.

Peter Barnes (barnes26@llnl.gov)



2 Proton radiographs of a tin metal plate accelerated by a high-explosive-driven shock. The assembly prior to detonation (**left**). Deformation of the accelerating plate and expansion of the explosive (**right**).

Novel Approach to Radiation Transport

The time-dependent transport of radiation through plasmas is important to the study of astrophysical phenomena, laser-produced plasmas, and thermonuclear weapons. In computational simulations, the transport equation for photons is coupled to time- and space-dependent equations describing properties of the plasma. The resulting system of differential equations can prove difficult to solve because of stiffness of the equations (often caused by the rapid variation of variables with spatial position or time or both) and the wide range of plasma opacities present in many problems. Deterministic methods, known as complete linearization and accelerated lambda iteration, remain the methods of choice for treating line radiation in stellar atmospheres, for example. On the other hand, Monte Carlo methods for radiation transport have advantages for problems involving fast temporal variation and geometric complexity not easily addressed by deterministic methods.

We developed and tested an innovative approach to solving the radiation transport in materials with high opacity. The technique uses symbolic implicit Monte Carlo, where the difference between the total radiation field and the material black-body radiation is propagated, symbolically, through the material [*Journal of Computational Physics* **189**, 330 (2003)]. Incorporating the new method into integrated simulation codes appears straightforward, because it involves a natural extension of currently used algorithms. Initial tests of our technique indicate orders of magnitude reduction in computational noise. Application of this method promises to substantially reduce

computation time for problems involving radiation transport through high-opacity plasmas, while increasing the accuracy of results.

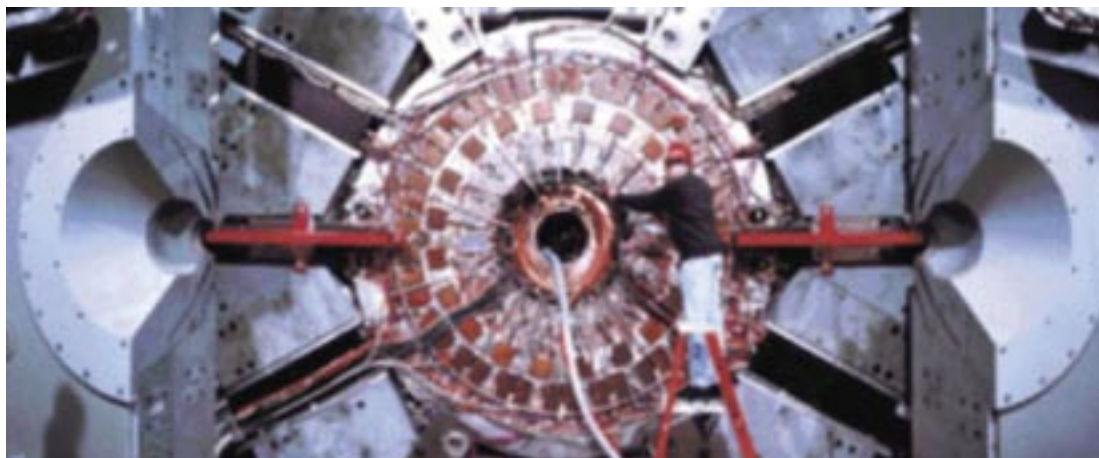
Eugene Brooks (brooks3@llnl.gov)

High-Energy Elementary Particle Research

N Division leads the Laboratory in the field of elementary particle or high-energy physics research. Physicists believe that a key to the disparity between the abundance of matter and antimatter in the universe lies in understanding an effect called charge-conjugation-parity (CP) violation. First observed in the 1960s, CP violation refers to the apparently small differences in the way that certain short-lived particles and their antiparticles decay. This violation of a fundamental symmetry may be responsible for the predominance of matter over antimatter in the universe.

The Laboratory participated in the design, construction, and commissioning of the B-Factory accelerator and the BaBar detector at the Stanford Linear Accelerator Center (Figure 3). The multiyear construction project, sponsored by the DOE Office of Science, involved a close collaboration among three California national laboratories—the Stanford Linear Accelerator Center, Lawrence Livermore, and Lawrence Berkeley National Laboratory. Since commissioning of the B-Factory, we have collaborated on physics experiments that unambiguously demonstrated CP violation in the B-meson system. The discovery and subsequent measurements have been a stunning confirmation of the Standard Model of high-energy physics [*Physical Review Letters* **89**, 201802 (2002)].

3 The BaBar particle detector at the B-Factory at the Stanford Linear Accelerator Center. The charge-conjugation-parity violation in B-meson decays was first discovered at the BaBar detector. The accelerator and the B-meson experiment are now performing well beyond the initial design goals. This opens the door to precision tests of the Standard Model of particle physics and the possibility of discovering new physics.



Our contributions were essential to the analysis leading to this discovery. We are actively participating in ongoing experiments that aim to measure other aspects of B-meson decays to further challenge the Standard Model [*Physical Review Letters* **91**, 071801 (2003)].

Doug Wright (wright20@llnl.gov)

Next Linear Collider

We are heavily involved in designing the Next Linear Collider (NLC), a mammoth accelerator that will be about 30 kilometers (km) long and cost roughly \$5 billion. As currently proposed, the NLC would house two opposing linear accelerators inside a 30-km tunnel, which would accelerate electrons and positrons—two elementary particles that are fundamental building blocks of the universe—to energies in the teraelectronvolt range (i.e., the equivalent of a trillion electronvolts). The interaction of the opposing beams of electrons and positrons will probe the origins of mass, space–time physics, and dark matter.

As part of the Stanford, Berkeley, Livermore, and Fermi national laboratory consortium working on the NLC, we have been actively developing plans to backscatter laser light from the high-energy beams in the collider, thereby converting the visible light to extremely high-energy gamma rays. If implemented, this development would enable study of collisions between extremely high-energy gamma rays. Livermore's strengths in accelerator technology, high-average-power lasers, and precision optics have been essential to formulating a plausible plan for this gamma–gamma collider option—an extremely complex and potentially far-reaching scientific and engineering challenge [*International Journal of Modern Physics A* **18**, 2921 (2003)].

Jeffrey Gronberg (gronberg1@llnl.gov)

Pioneering High-Energy Nuclear Interaction Experiment

We are actively involved in the Pioneering High-Energy Nuclear Interaction Experiment (PHENIX) at the premier high-energy nuclear physics facility, the Relativistic Heavy-Ion Collider at Brookhaven National Laboratory in New York. The goal is to identify the quark–gluon plasma, a form of matter believed to hold subatomic particles together. Collisions of high-

energy heavy ions at the collider re-create conditions that were present approximately 1 microsecond after the big bang. It has been predicted that the high-energy densities created in these collisions will cause a phase transition from protons, neutrons, pions, etc., into a plasma of quarks and gluons.

Lawrence Livermore has been a member of the PHENIX collaboration—an international effort—from the beginning. A team of Laboratory scientists and engineers designed much of the PHENIX analyzing magnet system and supervised its fabrication and testing. The system consists of a central magnet and two flanking muon magnets, sandwiched between plates of muon-identifier steel. The entire system stands more than three stories tall and weighs in excess of 2200 tons (Figure 4).

PHENIX researchers study collisions of bare gold ions at energies up to 200 gigaelectronvolts (GeV) per nucleon by monitoring the distribution and composition of decay particles that reach the detector. We are focusing on measuring the volume, lifetime, and violence of the collision zone. A large volume and long lifetime are some of the purported signatures of a quark–gluon plasma. To make these measurements, we have examined the production of pions, a two-quark particle, and analyzed their correlation. The more highly correlated the pions are in a given direction, the larger the volume of the collision zone in that direction. So far, we have found almost no elongation, in contradiction to most recent theoretical predictions [*Physical Review Letters* **89**, 82301 (2002)].

Because it is proving difficult to differentiate between signals resulting from the quark–gluon plasma and those that may be caused by other nucleon interactions in the gold–gold collisions, we are undertaking another experiment in an



4 Inside the Pioneering High-Energy Nuclear Interaction Experiment (PHENIX) detector. The central magnet is visible on the top. The south (left) and north (right) muon magnets are facing each other in the center. The muon tracking chambers are left of the south muon magnet, and a portion of the beam tube is visible right of the north muon magnet.

attempt to clarify the situation. We have installed a calorimeter at PHENIX to measure the fragments, and thus the number of interactions, resulting from the collision between a single proton or deuteron and the gold nucleus [*Physical Review Letters* **91**, 72301 (2003)]. These measurements will allow a proper analysis of results from nucleus–nucleus collisions, possibly enabling differentiation of the quark–gluon plasma signature.

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Search for Neutrino Oscillations

Cosmically created in stars and unleashed in nuclear reactors, neutrinos are one of the most pervasive forms of matter in the universe. However, they are also elusive and difficult to detect because the chargeless and seemingly massless neutrinos almost never interact with other forms of matter. Scientists now know that three types of neutrinos exist—the electron, muon, and tau neutrinos—and it has been theorized that they might be able to oscillate, or transform, into each other.

We are part of an international collaboration of 200 scientists from 26 institutions taking part in the Main Injector Neutrino Oscillation Search (MINOS) experiment centered at the Fermi National Accelerator Laboratory in Illinois to look for neutrino oscillations and begin to understand their particulars, which will improve understanding of particle physics and forces that guide the universe. A nearly pure beam of muon neutrinos generated at Fermilab will be directed at a detector deep in a former iron mine 735-km away (Figure 5). Fermilab will tune the beam to

an energy spectrum of 0.5 to 8 GeV, which, according to calculations, is the energy range that allows the most neutrino oscillations for the distance the beam needs to travel (735 km).

Researchers should see a decrease in the number of muon neutrinos that reach the detector and will be able to measure how many remain at each energy. The decrease will indicate that some of the muon neutrinos in the beam have changed into another type, and the oscillations will help confirm that neutrinos have mass. Physicists hope to uncover other details about the nature of neutrino oscillations, such as the oscillation probability (the fraction of a beam that can change from one type to another at a given energy) and oscillation length (distance a beam of neutrinos of a particular energy must travel to transform from one neutrino type to another and back again).

A key issue was how to design the 8-meter-(m) diameter steel planes of the detectors. Livermore engineers and physicists worked together to come up with a design that would allow sections of the 450-pound detector planes to be lowered into the mine through a 2- by 2-m shaft and assembled 800 m underground (Figure 5).

We are also a key participant in another MINOS-related effort to look at exactly what happens in creating the neutrino beam—or indeed, any beam of particles. The answers will have important ramifications for Livermore's science and stockpile stewardship research. We are leading the Main Injector Particle Production experiment—in collaboration with Fermilab and a group of 10 universities, colleges, and research institutes—to examine what happens when 120-GeV protons

5 Lawrence Livermore led the steel design for the Main Injector Neutrino Oscillation Search (MINOS) experiment. Scintillator modules were welded to octagonal steel planes—an 8-meter-diameter detector plane rests on the ground (center foreground), before it is raised into place to join the array of 450 planes that comprise the MINOS detector. Another detector plane in the raised position is visible behind it.



hit graphite targets. Beams of protons, kaons, and pions at energies from 5 to 100 GeV will also be generated to examine particle production on target materials as diverse as hydrogen and lead.

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Axion Experiment

N Division scientists have joined the University of California at Berkeley, the University of Florida, and the National Radio Astronomy Observatory to try to pin down the elusive axion particle, a long-sought relic from the first fractional second of the universe's birth and one of the most weakly interacting particles known. The collaboration intends to determine if the axion exists and if it constitutes a significant fraction of the universe's dark matter that we know is there but cannot see. The Livermore experiment is the only one in progress that can challenge recent theoretical estimates of axion mass and interaction strength.

The experiment is based on the theory that an axion, when it does interact, decays into two photons with frequencies in the microwave range of the electromagnetic spectrum. A major goal for our experiment is to increase the sensitivity of the measurements by increasing the sensitivity of the amplifiers and the size and magnetic-field strength of the cavity volume.

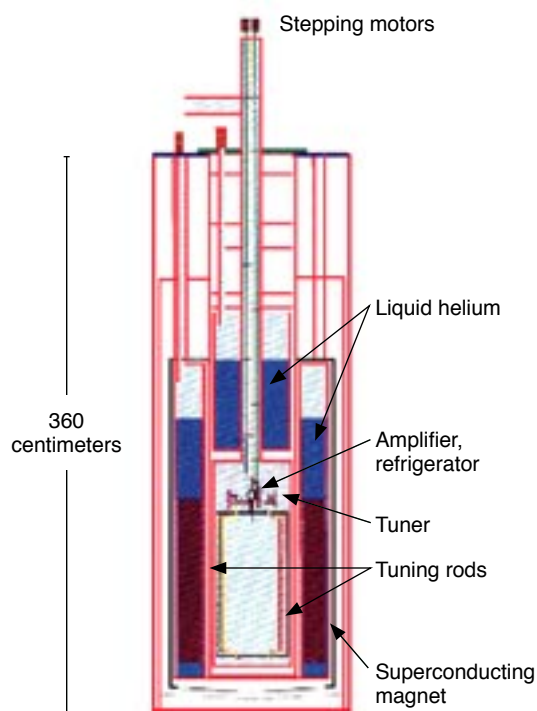
Whereas initial experiments elsewhere had microwave cavities the size of a small coffee can, the Livermore cavity—a copper-plated stainless-steel cylinder—is closer in size to an oil drum (Figure 6). The magnet's static magnetic field, which is used to coax axions into decaying, is about 200,000 times more powerful than Earth's magnetic field. Because the precise frequency of the axion decay is not known, the cavity resonance has to be tuned over the range of possible frequencies, from 0.3 to 3 gigahertz (GHz).

The Livermore experiment incorporates the latest technology for "hearing" any axion signals and separating them from noise. A very small excess of microwave photons above thermal and electronic noise levels would signal the decay of an axion. Because the expected signal from the decay of an axion is so faint, sensitive amplifiers are needed to boost the signal to detectable levels. The amplifiers used are based on the heterostructure field-effect transistor—an exotic semiconductor device

developed for military communications and now widely used by radio astronomers to amplify weak radio signals [*Reviews of Modern Physics* **75**, 777 (2003)].

The third generation of axion experiments will require more new technologies and techniques to further increase power sensitivity. These experiments will be able to detect axions even with the most pessimistic estimates of their coupling and will reach other parts of the frequency range not attainable with the current configuration. For this search, we will turn to a new type of radio-frequency amplifier based on a superconducting quantum interference device (SQUID). The new amplifier, which uses a direct-current SQUID made from superconducting niobium, can operate at frequencies well above 3 GHz—with record-low noise temperatures of 0.005 kelvin. Once this radio-frequency amplifier and its niobium SQUID are part of the experiment, the signal-to-noise ratio from axion decay will get a much-needed boost, which should make it possible to detect even the most elusive axion.

Leslie Rosenberg (rosenberg2@llnl.gov)



6 The axion experimental setup. An 8-tesla, 6-ton superconducting coil is wound around the outside of a copper-plated stainless-steel cylinder about the size of an oil drum. A set of tuning rods inserted into the cylinder's cavity is moved by stepper motors to tune the frequency of the cavity. Liquid helium cools the cavity, reducing the background noise. Amplifiers boost the faint microwave signal of the axion.



IGPP

INSTITUTE OF GEOPHYSICS AND PLANETARY PHYSICS

The Institute of Geophysics and Planetary Physics (IGPP) was founded in 1946 at the University of California at Los Angeles with a charter to “promote and coordinate basic research on the understanding of the origin, structure, and evolution of the Earth, the solar system, and the universe, and on the prediction of future changes as they affect human life.”

As a multicampus research unit of the University of California (UC) system, IGPP now has branches at UC campuses in Los Angeles, Irvine, San Diego, Riverside, and Santa Cruz, and at Lawrence Livermore and Los Alamos national laboratories. Because it is university-wide, IGPP has played an important role in establishing interdisciplinary research in earth and planetary sciences.

Each of the seven branches has a somewhat different scientific emphasis, reflecting the strengths of campus departments and laboratory programs. The IGPP branch at Livermore emphasizes research in tectonics and geochemistry in its Geosciences Center, and planetary science and astrophysics in its Astrophysics Research Center. It provides a venue for studying the fundamental aspects of these fields, thereby complementing other Livermore programs that pursue applications of these disciplines in national security and energy research. The Astrophysics Center is associated with the PAT Directorate.

The IGPP branch at Livermore, along with the one at Los Alamos National Laboratory, sponsors the University Collaborative Research Program (UCRP) to facilitate scientific collaborations among researchers at the campuses and national laboratories in areas related to earth science, planetary science, and astrophysics. This program provides funds for joint research projects involving UC researchers, other academic research centers, and the Laboratory. The goal of the UCRP is to enrich research opportunities for UC scientists by making available some of Livermore’s unique facilities and expertise and by broadening the scientific program at the Laboratory through collaborative work with campus researchers.

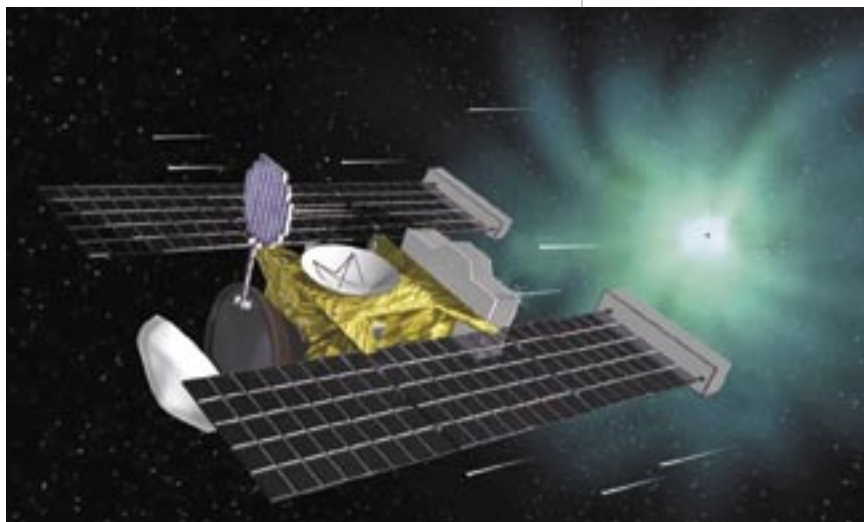
Although the permanent Livermore staff in IGPP is relatively small (at present four full-time employees), its two centers have become vital research organizations through their:

- Support of five resident postdoctoral fellows.
- Funding of about 20 UCRP projects each year.
- Hosting of a variety of visitors, guests, and faculty members from many institutions.
- Hosting of conferences, workshops, and seminars in astrophysics and geosciences.

Sample Return Center

We perform cutting-edge research on extraterrestrial nanoscale materials such as interplanetary dust particles (IDPs) collected in the stratosphere by ER2 high-altitude research aircraft used by the National Aeronautics and Space Administration (NASA). IDPs are complex, primitive solar system material that can provide information about the formation of organic matter in interstellar molecular clouds and the subsequent incorporation of such matter into our solar system. Results on isotopic anomalies observed in IDPs were recently published in *Science* [303, 1355 (2004)].

1 Artist rendition of the STARDUST spacecraft near the Comet Wild-2. A sample has been collected and stowed for return to Earth in February 2006.



We will also play a key role in investigating samples from the STARDUST mission, which was launched in February 1999 and will return to Earth in early 2006 (Figure 1). The primary purpose of STARDUST is to collect a dust sample from Comet Wild-2. Aerogel collectors on STARDUST were deployed to collect the sample on January 2, 2004. A secondary purpose is to collect samples of contemporary interstellar dust moving through the solar system in a stream parallel to the flow of interstellar gas.

NASA recently awarded the Laboratory \$3 million for the development of an advanced transmission electron microscope (named SuperSTEM) specifically for analyzing the STARDUST samples. In addition, STARDUST research will use other special analytical capabilities at Lawrence Livermore, including the new secondary-ion-mass spectrometer (nanoSIMS) and focused ion-beam instruments—housed in the Chemistry and Materials Science Directorate—as well as the Center for Accelerator Mass Spectroscopy.

The potential science return from the STARDUST mission is enormous. Apart from being the first US mission to collect and return a sample since 1972, analysis of even a few contemporary interstellar dust grains will greatly improve our understanding of the solid particulate composition of the interstellar medium and relative abundance of elements in interstellar

molecular clouds. Cometary grains will be similarly informative. Comets are unique, small icy bodies that spend most of their lifetimes at extreme heliocentric distances. They are believed to contain preserved interstellar dust as well as the first solids condensed in the inner solar system. Thus, cometary samples can be considered as “time capsules” from the earliest stages of solar system formation.

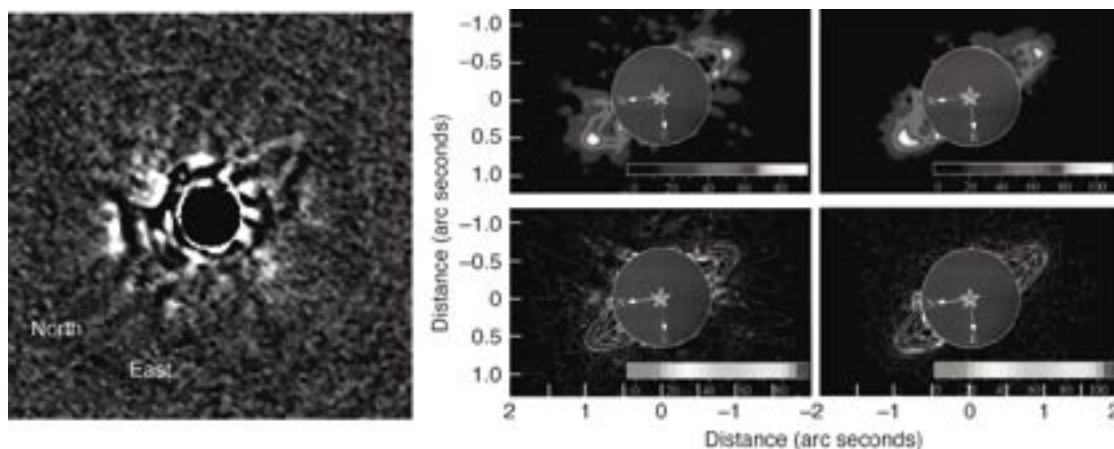
John Bradley (bradley33@llnl.gov)

Astrophysics Research Center

We deliver cutting-edge science and technology in pursuit of basic astrophysical knowledge. We focus on astronomical adaptive optics (AO), time-domain astronomical surveys, radio surveys, and the formation and evolution of structures in the early universe. These projects draw on and enhance Livermore’s capabilities in advanced detectors, remote sensing, advanced scientific computing, and high-energy and high-energy-density physics.

These research efforts have generated noteworthy accomplishments. The technology of AO and the incredible images obtained with it (surpassing those from the Hubble Space Telescope), the discovery of forming galaxies in the very early universe, and the creation of microlensing surveys have all been featured in newspapers and the scientific press. In 2003, we won more than 150 nights of major telescope

2 Close-up image of the young star HR4796 showing a tilted dust ring (**left**). The star is masked out by an occulting spot, and the image has been processed to highlight the ring, which results in white and black artifacts close to the star. The image was obtained with the Keck adaptive optics system at 3.8-micrometer wavelength. Near-infrared images of the dust ring obtained by Schneider et al. (**right**) using the Hubble Space Telescope [*Astrophysical Journal Letters* **513**, L127 (1999)]. Comparison of the Keck and Hubble images allow researchers to constrain the sizes of the dust particles in the ring and determine their origin.



time, significant observation time on a variety of satellites, and hundreds of hours of Very Large Array radio telescope time.

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Astronomical Adaptive Optics

Essential to astronomers today are AO systems that correct atmospheric aberrations of light coming into the telescope. These systems use mirror adjustments to remove Earth's atmospheric turbulence from the telescope's images, thereby producing unprecedented clarity. Lawrence Livermore has developed integrated AO and sodium-layer laser guide star systems and pioneered use of pulsed dye laser technology for use on large astronomical telescopes. The Laboratory's prototype astronomical AO system was installed at UC's Lick Observatory on Mount Hamilton near San Jose. The Laboratory then helped develop and install a larger AO system at the Keck Observatory atop Mauna Kea in Hawaii.

The AO system at the Lick Observatory has the only sodium laser guide star currently in operation. The 20-watt pulsed dye laser—developed by the Laboratory's Laser Programs—produces an eighth-magnitude artificial star. The system routinely achieves 0.5- to 0.15-arc-second resolution. A similar laser has been integrated into the Keck AO system. To further advance AO technology for astronomical observations, we have major roles in the National Science Foundation's Center for Adaptive Optics at UC Santa Cruz.

We use the AO systems at Lick and Keck in four scientific areas. The first is in "exploring" the solar system. Extremely high-resolution near-infrared images of solar system bodies can be taken from the ground, complementing rare and expensive spacecraft visits. Particularly interesting research includes measuring the shapes and sizes of asteroids, monitoring the evolution of weather on Titan or Neptune, and imaging the faint rings of Uranus or Neptune [*Astronomical Journal* **125**, 364 (2003)].

The second area involves investigations of one of the fundamental mysteries in astronomy: the nature and origin of supermassive black holes in the centers of galaxies. For these observations, the

Keck AO system is routinely achieving resolution equal to that of the Hubble Space Telescope.

The third area consists of studies of nearby active galaxies, including spectroscopic mapping of the merging nuclei of NGC6240 at 0.04-arc-second resolution.

The fourth area is the search for extrasolar planets. In collaboration with scientists at UC Los Angeles, we are using AO to search for planetary companions to young stars [*Astrophysical Journal* **581**, 654 (2002)]. Use of the Keck AO system permits detection of companions 1 million times fainter than their parent star, sufficient to detect a 10-million-year-old Jupiter-size planet through its thermal emission at near-infrared wavelengths. We are using a combination of Keck AO and Hubble observations to investigate dust rings surrounding young stars, which offer a favorable environment for planet formation (Figure 2).

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Bruce MacIntosh (macintosh1@lnl.gov)

Time-Domain Astronomical Surveys

Time-domain astronomy refers to investigations where the time dependence of astronomical phenomena is explicitly observed. Examples of recent interest include gamma-ray bursts and gravitational microlensing.

IGPP scientists continue to study the Milky Way's structure and composition by using the database from the Massive Compact Halo Objects (MACHO) Project. The MACHO Project used technology developed by Lawrence Livermore at the Mount Stromlo Observatory



3 A three-color composite image of objects in the Large Magellanic Cloud obtained by the Hubble Space Telescope. The source of the light in the microlensing event is the blue star near the center of the image, which is partially blended with a red object (indicated by the arrow) displaced by 0.134 arc second. The gravitational field of the object deflects the light as "seen" by the Hubble Space Telescope.

in Australia to monitor the universe over seven years for gravitational microlensing events, which occur when a massive object passes between a distant star and the observer.

While the MACHO Project finished monitoring the Large Magellanic Cloud (LMC) and central regions of the Milky Way galaxy at the end of 1999, analysis of the collected data continues, focusing on baryonic dark matter and mass distribution along the lines of sight. Recent results include an upper limit on the existence of dark clouds as a dark matter component of the galactic halo [*Astrophysical Journal* **589**, 281 (2003)] and the use of Hubble Space Telescope data to determine a location for most of the lenses seen in the LMC (Figure 3). Data mining of the MACHO database and follow-up observations have produced kinematic evidence for an old stellar halo in the LMC, suggesting that our galaxy and the LMC have similar early formation histories [*Science* **301**, 1508 (2003)].

We are also playing key roles in the next-generation microlensing survey of the LMC, known as the SuperMACHO Project. As part of this effort, we have been awarded 150 nights of observation time over five years on the Inter-American Observatory's 4-meter telescope (with a 64-megapixel mosaic camera) in Cerro

Tololo, Chile, to characterize the microlensing signals detected by the collaboration.

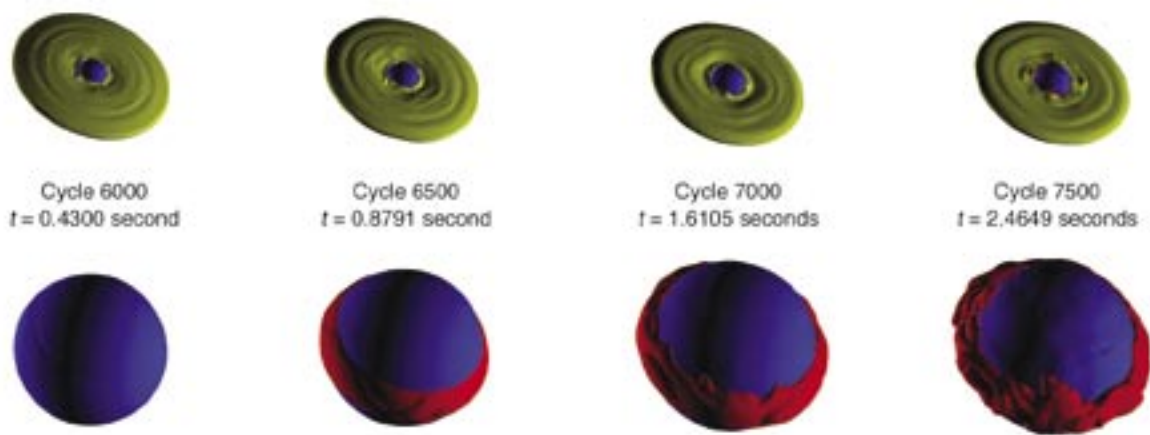
Finally, we are investigating the outer regions of the solar system to better understand the size distribution of material beyond Neptune. This material is thought to be relatively unprocessed from the time of the solar system's formation. We are collaborating with colleagues at two Taiwanese institutions to field the Taiwanese American Occultation Survey (TAOS), which will probe the density of small objects beyond Neptune by monitoring bright stars for occultations caused by these objects. The MACHO and TAOS projects would not have been possible without significant advances in automated telescope operation and data analysis.

Kem Cook (cook12@lml.gov)

Formation and Evolution of Structures in the Early Universe

In collaboration with colleagues from UC, NASA's Jet Propulsion Laboratory, and institutions in France, Italy, and the Netherlands, we are studying how the most massive galaxies formed in the early universe [*Astronomy and Astrophysics* **401**, 911 (2003)]. Using the two Keck telescopes and narrow-band filters, we have discovered gigantic emission-line halos and

4 Results from three-dimensional simulation of an accretion disk around a 1.2 solar mass, nonrotating white dwarf. Time (t) evolution (top) of a density contour of the accretion disk (yellowish green) and of the surface of the white dwarf (blue). Close-up of the white dwarf (bottom). The velocity field is initially discontinuous at the surface of the white dwarf (blue). A gradient develops, but the high-energy dissipation in this developing region ignites a ring of hydrogen (red).



large-scale structures associated with a number of such galaxies when the universe was only one billion years old. The origin of the halos is at present not understood. They may be caused by large “super winds” driven by enormous bursts of star formation or by primordial gas that is cooling for the first time since the big bang. Further spectroscopic observations and detailed computer simulations of the hydrodynamics and radiation processes in forming galaxies will be needed to unravel this mystery.

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Radio Surveys

Researchers at IGPP and UC Davis continue to extend the Faint Images of the Radio Sky at Twenty Centimeters (FIRST) survey and extract exciting new science from it [*Astronomical Society of the Pacific* **114**, 1359 (2002)]. FIRST is a high-spatial-resolution survey designed to produce the radio equivalent of the Palomar Observatory Sky Survey over 10,000 square degrees of the sky. To date, the FIRST catalog contains 135,000 radio sources and has led to the discovery of hundreds of new quasars, lensed quasars, and unusual radio galaxies. The database will be used to study not only quasars but also extragalactic radio emissions and cosmology. FIRST scientists have won a large amount of Hubble Space Telescope time to investigate further candidate lensed quasars identified by the FIRST survey.

Robert Becker (becker5@llnl.gov)

Djehuty Project

The scientific goal of the Djehuty Project is to develop the next-generation computer code for simulating stellar structure and evolution in three dimensions. The wide array of physical processes that must be treated and the complexity of fully three-dimensional calculations require significant advances in algorithms and access to large-scale, massively parallel computers. The Djehuty code and access to Livermore’s supercomputers will establish IGPP as a center

for stellar evolution study. In the future, Djehuty will become a user facility at IGPP, providing unique access to three-dimensional stellar modeling for the astrophysical community.

While the code is still in an experimental stage, we and our collaborators have begun modeling complex systems such as Keplerian accretion disks around a nonrotating white dwarf star and explosions in binary systems (Figure 4). Such modeling is directly relevant to the evolution of binary stars novae, and Type 1a supernovae.

The next phase in the development of Djehuty will focus on including a treatment of magnetic fields.

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I Division

OPTICAL SCIENCE AND TECHNOLOGY DIVISION

The Optical Science and Technology Division (known as I Division) supports existing Laboratory programs that are based on optical science and technology and advanced detectors, and collaborates on developing new programs for national security applications of optical and detector systems. As part of our mission, we also maintain and grow a strong science base in astronomical imaging and vision science.

Areas of general research and development in I Division include:

- Adaptive optics.
- Image processing and visualization.
- High-power laser systems.
- Optics and metrology.
- Multilayer technology.
- Photonics.
- Advanced detectors.
- Advanced intercept technology.

Adaptive Optics

The Adaptive Optics (AO) Group in I Division develops and tests a broad range of advanced wave-front control technologies. Current applications focus on:

- Remote sensing.
- High-power lasers.
- Astronomy.
- Human vision.

In the area of remote sensing, a large collaboration led by Livermore scientists successfully completed the Coherent Communications, Imaging, and Targeting (CCIT) Program, supported by the Department of Defense's Defense Advanced Research Projects Agency. The goal was to develop powerful, new capabilities for secure, free-space communication links and for aberration-free, long-range three-dimensional imaging and targeting. The fundamental enabling technology was innovative spatial-light modulators (SLMs) based on microelectromechanical systems (MEMS), which provide a quantum leap in advanced photonics components and high-speed electronics for wave-front control.

Phase I of the CCIT Program, which lasted two years, was executed by a team of researchers from Livermore, four universities (Boston University, Stanford University, University of California at Berkeley, and Georgia Institute of Technology), several MEMS/photonics companies (Boston Micromachines, MicroAssembly Technologies, and Lucent Technologies), and major US aerospace companies (Ball Aerospace, Boeing, Harris, HRL Laboratories, Lockheed Martin, Northrop Grumman, Raytheon, TRW, and Aerospace Corporation). The CCIT Program successfully culminated in 2003 with the field test of a 1024-element MEMS SLM (Figure 1), which was used to correct a laser beam propagating over a 1.5-kilometer (km) horizontal path. The success of phase I research and development led to a phase 2 effort, headed by Lucent Technologies, to develop a MEMS SLM product line suitable for field use by the military.

Another project in the AO Group is a collaborative effort with the Laboratory's Nonproliferation, Arms Control, and International Security Directorate on enhanced surveillance imaging. The goal is to use advanced image processing techniques to improve the resolution of images, such as personnel, vehicles, and buildings, taken over horizontal or slant paths with ranges from about 1 to 100 km. Image reconstruction of these generalized scenes over long slant ranges is notoriously difficult, but work in 2003 demonstrated an order of magnitude improvement in image quality for a variety of scenarios using a simple, modular, portable system with a 30-centimeter (cm) optical aperture (Figure 2). Work in 2004 will focus on extensions of these techniques to fast-moving targets.

In the area of high-power lasers, I Division and the Laboratory's Laser Science and Technology Program are collaborating on development of a solid-state, heat-capacity laser. Supported by a contract with the US Army, this project uses an AO system inside an unstable resonator cavity to compensate for optical aberrations in the laser-gain media. These aberrations lead to

degradations in beam quality that limit the ability to bring the beam to a sharp focus on a target. In 2003, the team successfully demonstrated this adaptive resonator approach (originally proposed in the 1980s) for the first time and verified its full functionality for maintaining beam quality of the 10-kilowatt (kW) laser system at high powers. The system will be fielded at the Army's High Energy Laser Test Facility in White Sands, New Mexico. Currently, the Laboratory is building a new, compact 40-kW laser that will use diode technology in place of flashlamps to pump the solid-state laser medium.

In astronomy, we are a major participant in the National Science Foundation Center for

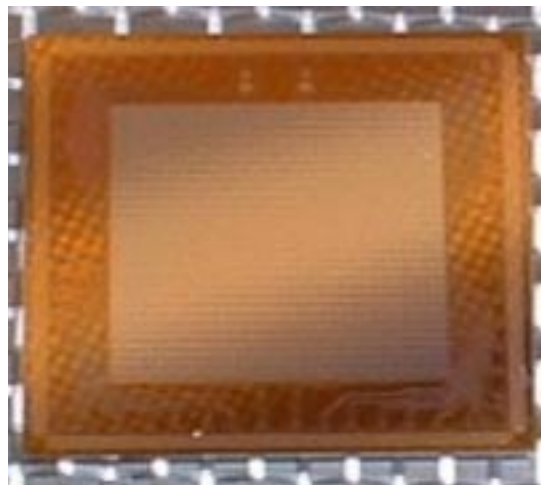
Adaptive Optics (CfAO) headquartered at the University of California at Santa Cruz. Founded in 1999, the CfAO includes 11 university nodes around the country, 10 national laboratories and observatories, and over 20 industrial partners. The CfAO supports research on AO for extremely large telescopes as well as on extreme AO for detection and characterization of extrasolar planetary systems [*Proceedings of SPIE* **4854**, 554 (2003)].

In 2003, work on AO for extremely large telescopes focused on design concepts for a multiconjugate AO system for a 30-meter (m) telescope. The Thirty Meter Telescope Project recently received \$35 million from the Gordon and Betty Moore Foundation for preliminary design work, including the AO, and we are actively involved in this effort.

The goal of our research on extreme AO is to develop the world's most powerful AO system for an existing 8- to 10-m telescope, with new capability for the high-contrast imaging required for detection and characterization of planetary systems around nearby stars. Several technical advances were made for the design of this instrument in 2003 (Figure 3), and a full conceptual design is now in progress.

We continue to support operation of the world's only fully functional laser guide star AO system, on the 3-m telescope at the University of California's Lick Observatory. A major upgrade of the AO control system was accomplished in 2003 [*Proceedings of SPIE* **4839**, 354 (2003)]. In addition,

1 The first 1024-pixel microelectromechanical-systems-based spatial light modulator delivered by Boston University and tested at Livermore met its performance goals. Each pixel (or individual spatial light modulator) can be individually controlled. This device was used in a successful field demonstration in which it corrected the atmospheric distortion of the wave front of a 1.55-micrometer-wavelength laser beam propagating over a 1.5-kilometer horizontal path.



2 Demonstration of enhanced surveillance imaging over a 1.5-kilometer horizontal path at sunset using an image intensifier. The image on the right was enhanced using newly developed bi-spectral image processing algorithms.



we participated in commissioning of the laser guide star AO system on the 10-m Keck telescope in Hawaii. The first tests of this system, built collaboratively by Livermore and Keck Observatory in a project begun in 1994, were conducted successfully in October 2003 (Figure 4). The first scientific observations are scheduled for fall 2004.

In the area of human vision, we successfully developed a MEMS-based AO phoropter (MAOP) with support from the Department of Energy Biomedical Engineering Program [*Proceedings of SPIE* **5001**, 50 (2003)]. In time, MAOP may replace the traditional phoropter used by ophthalmologists and optometrists to examine eyes and prescribe corrective lenses, laser refractive surgery, and other vision correction technologies currently under development. The MAOP lets patients immediately see how objects actually look (without distortion), allowing clinicians to more accurately adjust prescriptions. The Laboratory research team received a 2003 R&D 100 Award for the development of this innovative eyesight-correction system. Livermore's partners in the MAOP Project included Sandia National Laboratories, University of Rochester, University of Southern California (USC), University of California at Davis, University of California at Berkeley, the US Army Aeromedical Research Laboratory, Bausch & Lomb, and Wavefront Sciences.

The AO Group is also part of a team, led by the University of Rochester, selected by DOE for a five-year Bioengineering Research Partnership to develop AO instrumentation for advanced ophthalmic imaging. In this partnership, Livermore will develop a portable MEMS-based AO scanning-laser confocal ophthalmoscope for the Doheny Eye Institute at USC. This instrument will give ophthalmologists an unprecedented, cellular-level view of the retina in a clinical instrument, which will aid in diagnosis and treatment of blinding eye diseases.

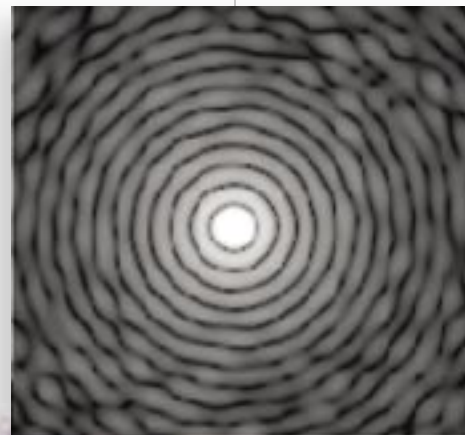
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Extreme Ultraviolet Lithography

Livermore is supporting the semiconductor industry

in developing extreme ultraviolet lithography (EUVL) for fabricating integrated circuits on chips with feature sizes smaller than those attained using traditional laser-based lithography. Since 1997, the Laboratory has joined with Lawrence Berkeley and Sandia national laboratories under an umbrella partnership called the Virtual National Laboratory. The goal of the Virtual National Laboratory is to experimentally demonstrate that lithography can be achieved using light with a wavelength of about 13.4 nanometers (nm), which is more than a factor of 10 shorter than that used currently. Livermore has led development of the projection optical system used to image the circuit pattern on the mask—the light-sensitive resist coating—on the wafer. The Laboratory has also been responsible for identifying a way to fabricate the mask without defects that cause the printed circuit to have errors and degrade performance [*Proceedings of SPIE* **5037** (2003)]. These challenging tasks required many unique skills including knowledge of x-ray optical systems, precision engineering, multilayer coating, and interferometry.

The projection optics designed and built at Livermore constitute the most accurate imaging system ever constructed, with an average wave-front error of about 0.8-nm root-mean-square (rms) over the extended area of the circuit being imaged.



3 The extreme adaptive optics, high-contrast imaging testbed (**bottom**) will aid in developing the world's most powerful adaptive optics system for an 8- to 10-meter telescope, with new capability for high-contrast imaging. The testbed uses the world's most accurate interferometer technology, which was developed at Lawrence Livermore, and the image obtained with it (**top**) demonstrates greater than 10^6 contrast.

In 2003, this imaging system was installed in a prototype EUVL system at Sandia. The EUVL tool was successfully tested and won an R&D 100 Award (including Editor's Choice Award) in 2003. The quality of the imaging system played a key role in the Virtual National Laboratory's lithography demonstration and is a testament to the tremendous collaboration among three Laboratory directorates (PAT, Engineering, and Chemistry and Materials Science) and external partners.

In 2003, I Division's interferometry team and Engineering's Precision Engineering Group collaborated on the alignment of a small-field EUV camera, known as the Micro-Exposure Tool, that will be used for exposures to develop resists. The collaboration successfully overcame a number of technical challenges associated with this two-mirror camera and delivered an optical system that yielded yet another new record for lowest wave-front error—0.56-nm rms. This outstanding performance would not have been possible without concurrent development of new interferometry methods. In 2003, we also began development of lensless phase-shifting diffraction interferometry. In this technique, a test beam illuminates an

optic to be tested and then combines it with a reference beam to form diffraction fringes. The amplitude and phase of these diffraction patterns are collected by a charge-coupled-device camera, without any lenses for imaging the test optic onto the camera, as is typical for other interferometers. Special algorithms were developed for using the phase and amplitude information to infer what errors in the optic led to the particular patterns recorded on the charge-coupled device. This new technique, in combination with the availability of 64-bit microprocessors, will enable measuring optical systems with an accuracy better than 100 picometers.

The fabrication of the mask is also one of the Laboratory's responsibilities and presents one of EUVL's major challenges. The mask is the "picture" of the desired circuit pattern that is imaged onto the wafer. If there are any defects such as particles on the mask, then these will be printed on the wafer and will likely render the circuit unusable. Livermore is currently pursuing three broad strategies for reducing defects. Each of these strategies is strongly dependent upon developing a better fundamental understanding of the deposition process.

4 The successful October 2003 test of the complete Keck laser guide star adaptive optics system, built collaboratively by Livermore and Keck Observatory. The yellowish laser beam emanating from the Keck II telescope (center) is visible against the night sky. (Photo credit: John McDonald, Canada-France-Hawaii Telescope Facility.)



One approach, which also won an R&D 100 Award in 2003, is developing a planarization process that smoothes defects during coating, thus rendering them unprintable. This procedure, which has been tested in experiments where gold nanoparticles have been placed on substrates prior to deposition of the multilayer, has successfully reduced 70-nm-high bumps on the top surface to less than 1 nm (Figure 5). By modeling the effects of the multilayer stack on the image created at the wafer plane, the researchers have demonstrated that defects on the 1-nm scale are unprintable.

Another approach is based on modifying the geometry or physical properties of the multilayer in the vicinity of a defect, so that it is optically invisible to the lithography process [*Proceedings of SPIE* **5037**, 5750 (2003)]. The goal is to develop a repair process that can mitigate a small number of defects, thus offering another opportunity to improve the production yield of masks. Finally, we are using first-principles models to understand the physics that govern the transport of particles within the coating tool. The aim is to define particle trapping strategies that reduce the probability that a particle reaches the mask during coating. The development of deposition tools that produce a reduced number of defects, combined with a variety of mitigation strategies, offers a promising path to meeting the commercial production requirements for defect-free masks.

The Cooperative Research and Development Agreement between the Virtual National Laboratory and the EUV Limited Liability Corporation formally came to a close in December 2003. Although the Virtual National Laboratory is heralded as having identified all key technical risks of EUVL and proposing roadmaps for resolving these risks, further research and development activities are required before commercial equipment can be designed for all aspects of chip production. In 2004, Livermore's EUVL program will continue to focus on the development of optical systems and the reduction of mask defects under work for others contracts with commercial companies and the International SEMATECH Consortium.

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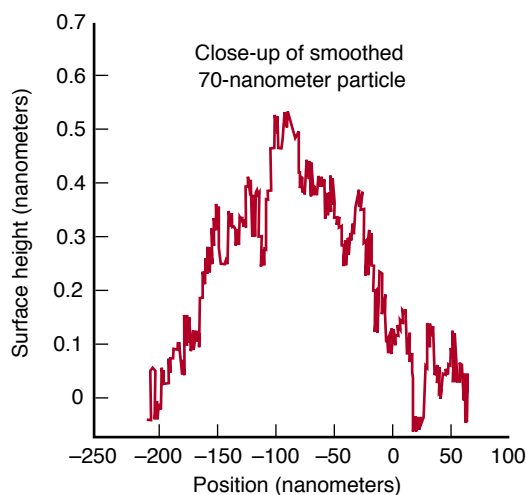
Linac Coherent Light Source

The Linac Coherent Light Source (LCLS) is a collaboration between the Stanford Linear Accelerator Center, Lawrence Livermore and Argonne national laboratories, and the University

of California at Los Angeles to build the world's first x-ray free-electron laser at Stanford under the sponsorship of the Department of Energy Office of Basic Energy Sciences. After the start of operations—currently planned for 2008—LCLS will provide x-ray beams of unprecedented brightness, delivered in femtosecond pulses, with full transverse coherence. Potential for scientific impact will be great in fields that range from materials science to chemistry, atomic and molecular physics, and structural biology.

We are responsible for developing the x-ray transport, optics, and diagnostic systems for the LCLS Project [*AIP Conference Proceedings* **641**, 596 (2002)]. Most of the work in 2003 involved project-planning activities, including development of the project baseline, in support of the Critical Decision-Two milestone that would authorize construction to begin in fiscal year 2006.

In parallel with construction planning, we are investigating the feasibility of single-molecule imaging experiments on the LCLS. Ultrashort x-ray pulses from LCLS offer the potential for imaging noncrystalline biological (and other) materials at atomic resolution. For proteins, simulations based on molecular dynamics and hydrodynamics models indicate that if very short x-ray pulses (100 femtoseconds or less) with sufficient photons per pulse ($\sim 10^{12}$) are available, a scattering pattern can be recorded from a single protein molecule in the gas phase before radiation damage manifests itself and ultimately destroys the molecule. In a process akin to single molecule cryo-electron microscopy, thousands of images could be recorded, aligned, and averaged, and a three-dimensional tomographic reconstruction



5 Profile of the top surface of a multilayer stack after planarization treatment of a 70-nanometer-high defect, which was caused by placing gold particles on the substrate prior to coating.

would lead to the atomic-level structure of the protein molecule. We have developed several algorithms that reconstruct an image based on the measured coherent x-ray diffraction pattern and have successfully tested them on data acquired at the Advanced Light Source at Lawrence Berkeley National Laboratory [*Physical Review Letters* **91**, 203902 (2003)]. The reconstructed images are the highest resolution x-ray images of a nonperiodic object ever obtained, and work on performing the full three-dimensional reconstruction from experimental data is under way (Figure 6). In addition to formulating hydrodynamic models of the radiation damage, we are designing a suite of experiments to validate the models' predictions of the interaction of molecules with intense x-ray pulses. These experiments will be carried out at the Short-Pulse Photon Source at the Stanford Linear Accelerator Center and the Tesla Test Facility at Deutsches Elektronen-Synchrotron in Hamburg, Germany.

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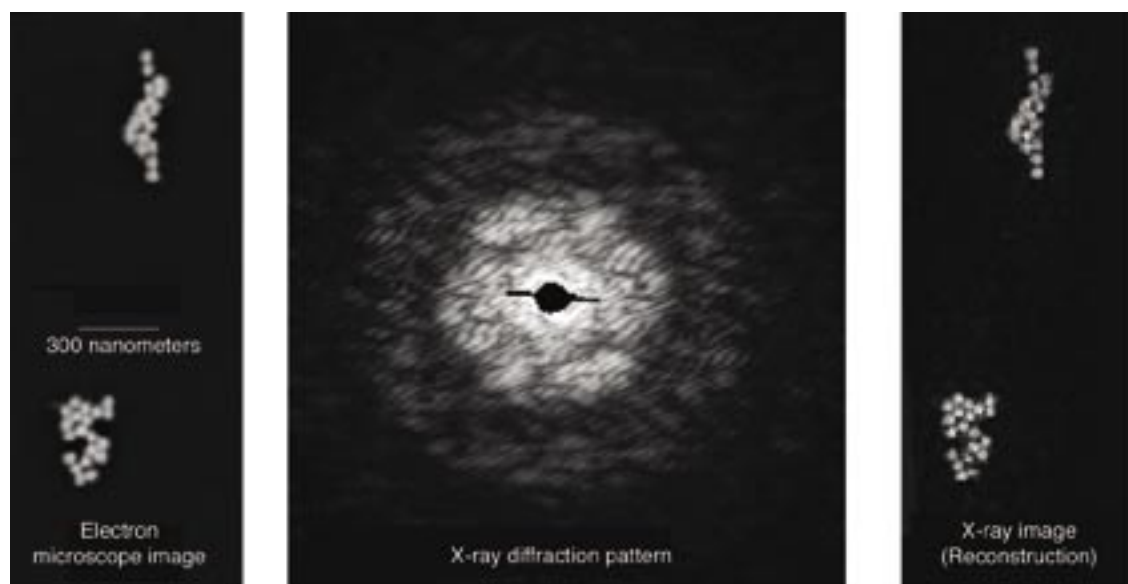
Advanced Detectors

The Advanced Detector Group is developing high-resolution and high-sensitivity detectors for use in several spectral regions from the near-infrared to gamma-ray wavelengths. At x-ray wavelengths, the detectors combine high-spectral resolution with high efficiency over a wide

energy band. Such detectors are ideal for both astronomical measurements and synchrotron-based spectroscopy of biological samples. At gamma-ray wavelengths, the detectors can measure the ratio of one nuclear isotope to another, with high precision, for nonproliferation and arms control applications.

Work was completed on the High-Energy Focusing Telescope (HEFT), a hard x-ray observatory that will fly on a high-altitude scientific balloon in 2004 to observe emissions from supernova remnants, supermassive black holes, and the center of our galaxy. HEFT, which is sponsored by the National Aeronautics and Space Administration (NASA), is a collaboration involving Columbia University, Lawrence Livermore, California Institute of Technology, and the Danish Space Research Institute [*Proceedings of SPIE* **4851**, 607 (2003)]. Research and development on HEFT produced a number of spinoff benefits in the past year—it was proposed to NASA for a small explorer satellite known as NuSTAR, and has now been selected for detailed phase A study. The HEFT detector concept is the core of a new radiation detection system, known as RadNet, the development of which is funded by the Department of Homeland Security. The RadNet units use the basic HEFT electronics and detector concept, packaged inside a cellular telephone, to provide a widespread network of

6 Reconstruction from a coherent x-ray diffraction pattern. An electron microscope image of the test object, which consists of 50-nanometer-diameter gold spheres arranged on a membrane (**left**). The coherent diffraction pattern recorded at a wavelength of 2 nanometers (**middle**). This was processed with a novel algorithm, called “shrinkwrap,” to produce the reconstructed image of the test object with a resolution of 10 nanometers (**right**). The experiments were performed in collaboration with Malcolm Howells (Lawrence Berkeley National Laboratory) and John Spence (Arizona State University).



low-cost, portable radiation detectors for law enforcement and emergency responders.

The move of the Measurement Sciences Group from Lawrence Berkeley National Laboratory to Lawrence Livermore was completed in 2003. The germanium detector fabrication facility is now fully functional in new laboratories at Livermore. In 2003, the facility produced over 20 working detectors and developed a new type of detector using amorphous germanium. These germanium-based detectors are now being used in Compton imagers that have broad applications to radiation detection problems in the area of nonproliferation of nuclear materials and devices (Figure 7).

We are continuing to apply superconducting materials and low-temperature techniques to the development of cryogenic detectors for gamma-ray and neutron spectrometers [*IEEE Transactions on Applied Superconductivity* **13**, 643 (2003)]. This effort has led to some of the highest resolution hard x-ray detection systems available. The high spectral resolution, increased sensitivity, and high-energy response allow heretofore impossible measurements on the isotopic composition of nuclear materials. These cryogenic detectors have a broad range of scientific and programmatic applications ranging from biomedical imaging to nuclear forensics.

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Advanced Interceptor Technology

The Advanced Interceptor Technology (AIT) Program is supporting the Missile Defense Agency in developing advanced propulsion technologies needed in the next generation of ground- and sea-based kinetic interceptor vehicles, which are designed to shoot down enemy ballistic missiles during their boost and ascent phases of flight. These technologies are also considered essential in space-based interceptor applications.

The AIT Program is using nontoxic propellants based on hydrogen peroxide and kerosene that offer "safe" operation in manned environments such as on a ship or submarine. In addition, a pump-fed propulsion design has significant mass savings over conventional approaches for very high-performance vehicle systems. A divert and attitude control system that uses small thrusters, which are fed pumped propellants, is under development for the Missile Defense Agency



7 A large germanium-strip detector produced in new laboratory facilities at Lawrence Livermore, which house research of the Measurement Sciences Group, formerly of Lawrence Berkeley National Laboratory. This one-of-a-kind facility allows all germanium detector processing, contacting, and testing to be done in a single laboratory.



8 A recent interceptor testbed vehicle as it "flies" on the outdoor 40-meter test rail at Lawrence Livermore (**top**) and during inspection prior to an experiment (**bottom**). This lightweight (~30-kilogram mass) vehicle demonstrated ~0.5-g acceleration using new, nontoxic hydrogen peroxide thrusters and a lightweight pump assembly.



Advanced Systems Office. Results to date indicate that vehicles with a mass of only 30 kilograms should be able to achieve velocity changes of up to 2.5 km per second (Figure 8). This technology also could be used for a number of future NASA planetary missions, such as the Mars sample return mission, where pumped propulsion appears to be very promising. These missions offer an exciting and demanding challenge that we can support.

While working on advanced propulsion technology, the AIT Program has developed several unique engineering testbed vehicles and dynamic air-bearing test capabilities that enable high-fidelity ground experiments, such as four-degrees-of-freedom intercept maneuvers on an air rail as well as five-degrees-of-freedom docking experiments on an air table. Recent rail tests have successfully demonstrated the performance of a ground test vehicle with its pump-fed propulsion system (Figure 8).

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ILSA

INSTITUTE FOR LASER SCIENCE AND APPLICATIONS

Created in 1996, the Institute for Laser Science and Applications (ILSA) contributes to the science of laser interaction with matter and advanced laser technologies—two areas important to the Laboratory. We support collaborative research on applications of high-intensity, high-energy lasers in:

- High-energy-density science, including laser fusion physics and astrophysics.
- Physics of laser-driven plasmas.
- Matter created with ultrahigh-intensity (petawatt) lasers.
- Advanced plasma diagnostics.
- Novel x-ray sources.
- Photon–matter interaction science using advanced light sources.

We facilitate training and research for university students and faculty with our program of outreach to the university community, through the University Collaborative Research Program and organizing conferences and workshops in topical areas of interest to the laser and plasma science communities. Our work is carried out in collaboration with colleagues from various Livermore programs having common research interests as well as with faculty and students from University of California (UC) campuses and other universities with unique laser or other high-energy-density facilities.

PLEIADES Compton Scattering X-Ray Source

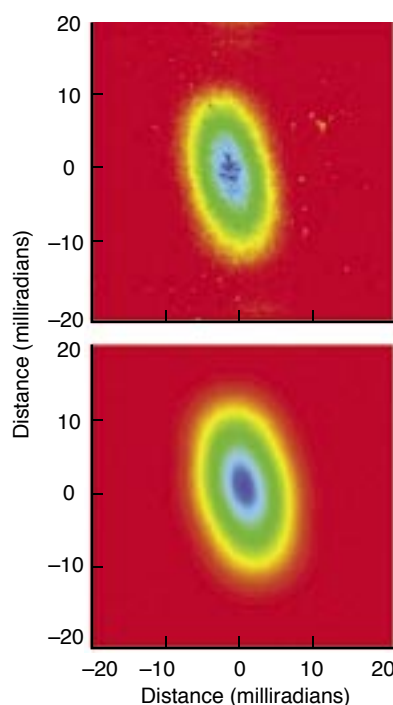
ILSA scientists have made key contributions in developing a novel, short-pulse x-ray source with very high brilliance. PLEIADES (Picosecond Laser Electron InterAction for the Dynamic Evaluation of Structures) couples the existing 100-megaelectronvolt electron linear accelerator, upgraded with a novel low-emittance electron source, to a 35-femtosecond pulse laser. The x rays are generated by scattering of laser photons from the high-energy electron beam produced by the accelerator.

In commissioning experiments using a detector with a cooled charge-coupled device and cesium iodide scintillator, we observed hard, near-monochromatic x rays. The photon energy

was approximately 70 kiloelectronvolts, and the observed angular distribution of the x rays agreed well with the three-dimensional code prediction used to model the interaction of laser photons with relativistic electrons (Figure 1).

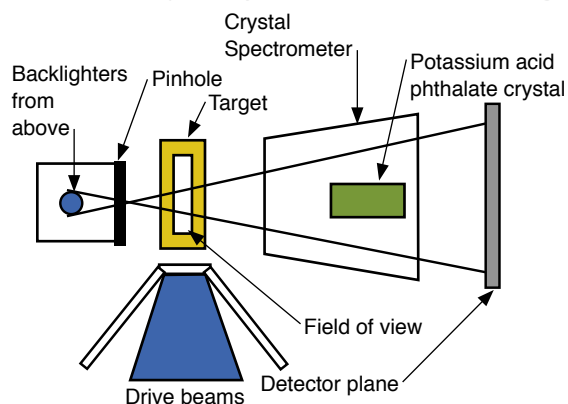
The new capability provided by PLEIADES will enable scientific and technological advances in several areas, including dynamic materials studies on sub-picosecond timescales for stockpile stewardship and development of laser-driven, compact, tunable x-ray sources for diverse applications that range from advanced diagnostics for the National Ignition Facility to protein crystallography. PLEIADES can also serve as a testbed for demonstrating new x-ray techniques required for experiments planned at fourth-generation light sources, such as the Linac Coherent Light Source at the Stanford Linear Accelerator Center, which will become available over the next several years.

Several potential applications of PLEIADES require optimizing further the brightness of the short-duration x rays produced. We



1 Image obtained with a charge-coupled device showing the spatial distribution of the PLEIADES x rays (**top**), and the theoretical x-ray angular distribution from the three-dimensional code (**bottom**). The agreement between theory and experiment is excellent.

2 Schematic of the experimental setup viewed from above for the Radiative-Shock Testbed (not to scale). The target consists of two slabs: polycarbonate plastic (60-micrometers thick) and silica aerogel foam (2000-micrometers thick) separated by a 150-micrometer vacuum gap. The target is contained inside a gold tube (shown in gold), which has two windows on the sides for diagnostic access. The laser beams (shown in blue) strike the plastic slab and the laser-matter interaction hydrodynamically drives the radiative-precursor shock in the foam. Additional laser beams strike the backlighter, which produces x rays used to diagnose the target.



are investigating, both theoretically and experimentally, the interaction of relativistic electrons and coherent photon fields in vacuum. One purpose is to establish a theoretical formalism capable of fully describing the three-dimensional nature of the interaction as well as the effect of the electron and laser beam phase-space topologies on the x-ray spectral brightness. Another is to explore Compton scattering as a source of tunable x rays for enabling high-throughput protein crystallography.

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Radiative-Shock Testbed

Radiative precursor shock occurs when the flux of ionizing photons radiated forward from a shock front exceeds the flux of atoms approaching the shock front. A dramatic example of radiative shock occurs in the impact of Supernova 1987A ejecta on the material surrounding the supernova (called the circumstellar ring nebula). Radiative shocks also occur in nuclear explosions and some inertial confinement fusion plasmas. The computational simulation of such shocks is difficult because a multitude of physical effects must be described accurately, and there is very little laboratory experimental data available for testing various models.

To address this problem, Livermore researchers have been developing the Radiative-Shock Testbed, in collaboration with colleagues from the University of Michigan and University of Rochester. The focus is to optimize target designs for high-energy laser experiments that can produce the high-quality data needed to benchmark computational models of radiative shocks. The research involves synergy between astrophysical phenomena involving shocks, modeled with a computer code currently under development, and the physics of a proposed inertial confinement

fusion ignition capsule, which uses a radiative shock in xenon gas. The initial phase of the project was funded by Livermore's Laboratory Directed Research and Development Program and involved four graduate and five undergraduate students at the University of Michigan.

In experiments at the Omega laser at the University Rochester, we observed a radiative precursor shock in a hydrodynamically driven system (Figure 2). The peak temperature and length of the radiative precursor were found to depend sensitively on the laser drive power. The data were consistent with a simple estimate of a threshold shock velocity required to produce a radiative precursor. Results were published jointly by University of Michigan, Lawrence Livermore, and University of Rochester researchers [*Physical Review Letters* **89**, 16503 (2002)].

This research collaboration with the University of Michigan was the driver for a 2003 sabbatical at Livermore by Professor Paul Drake, accompanied by two of his graduate students. The sabbatical was managed through the University Relations Program and co-sponsored by Livermore's National Ignition Facility Programs Directorate and ILSA.

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Modifying Glass with Ultrashort Laser Pulses

We are conducting research on using ultrashort laser pulses to modify optical properties of glass, a technique that offers new ways of making integrated waveguide devices. One such device is an integrated frequency-doubled waveguide laser. Others include curved waveguides, splitters, and interferometers.

When glass is irradiated with femtosecond pulses of a near-infrared laser light, energy is deposited in the glass through multiphoton ionization, avalanche ionization, and the subsequent transfer of energy to the lattice. The result is localized changes in the density and the refractive index of the glass. Measurements of the fluorescence from the exposed region indicate that color centers are also formed. By using appropriate geometry of laser focus and moving the glass sample at a constant speed perpendicular to the laser beam during irradiation, we can form an elongated groove or a channel in the glass that acts as a waveguide.

While the mechanism of energy deposition induced by femtosecond laser pulses are thought to be the same for different types of glasses, we have found that the spatial distribution of refractive index changes is different for fused silica and phosphate glasses [Applied Physics Letters **82**, 2371 (2003)]. In fused silica, both waveguiding and defect formation occur in the same region, at the focal point of the laser beam. This means that deposition of the laser energy results in a material with a higher density and refractive index. For phosphate glass, the data suggest that the femtosecond laser beam induces a modified region in the focal spot that has a lower density and refractive index than the initial glass. Color centers are also created in this central region. On the other hand, higher refractive index regions, which function as waveguides, are formed around the central area irradiated by the laser. We believe the higher refractive index material results from stress created by the expansion of the laser-irradiated, central region. The fact that color centers are not found in the waveguide regions lends supporting evidence that the waveguides are not created via direct exposure to the laser beam.

This area of research has attracted five graduate students from the Department of Applied Science at UC Davis (Figure 3) and has recently led to six refereed journal articles, five contributed conference proceedings papers, and four invited conference talks. One of the five graduate students was awarded the Norbert J. Kreidl Award for Young Scholars by the Glass and Optical Materials Division of the American Ceramic Society and went on to become a postdoctoral employee in PAT. Another student won the Best Student Poster Competition in the 2003 Conference on Commercial and Biomedical Applications of Ultrafast Lasers, SPIE Photonics West, San Jose, California. A third graduate student recently joined Harvard University as a postdoctoral researcher.

Denise Krol (dkrol@llnl.gov)



3 Institute for Laser Science and Applications students James Chan (left), now a PAT postdoctoral researcher, and Rafael Leon align a laser as part of a confocal microscopy setup used to investigate the spatial distribution of refractive index changes in glass induced by femtosecond laser pulses.

University Collaborative Research Program

We participate in the Laboratory's University Collaborative Research Program by providing support for research collaborations in the form of "mini grants." The goal is to encourage university research that could significantly impact laser science and laser science application topics in support of the Laboratory's missions and to train future Laboratory employees and faculty members in these areas. The range of research topics is illustrated in the table on p. 50, which lists the projects funded by ILSA at a nominal \$30,000 each in fiscal year 2003. All of these projects involve at least one graduate student doing PhD research under the supervision of each campus principal investigator listed. In several cases, the graduate student's research involves the use of PAT laser facilities.

To capture the depth and breadth of ILSA's research partnership portfolio, we detail two of the eight projects listed in the table, covering research in high-energy-density science exploring fast electron production and energy transport (see Investigations of Energy Transport in Over-Dense Material Initiated by Ultrashort Pulse, High-Energy Laser Pulses) and photon-matter interaction science for medical applications (see Laser Spectroscopy for Evaluation of Transplant Tissue Viability and Early Detection of Rejection).

Don Correll (correll@llnl.gov)

Investigations of Energy Transport in Over-Dense Material Initiated by Ultrashort-Pulse, High-Energy Laser Pulses

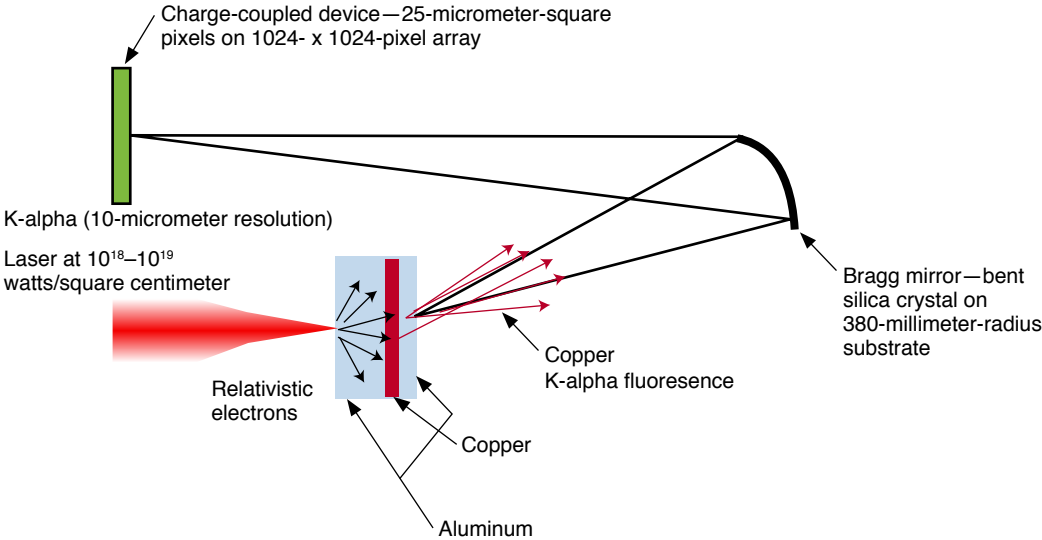
We investigated electron transport within solid-density targets irradiated by light from high-intensity, short-pulse lasers (Figure 4), including the JanUSP laser operated by PAT at Livermore; the Vulcan laser at Rutherford Appleton Laboratory, Chilton, United Kingdom;

and the Gekko facility at the Institute for Laser Engineering, Osaka University, Japan. Because fast electrons can knock out an inner shell electron—depending on factors such as laser power deposited, actual energy of the fast electron, and nature of target material—the consequent K-alpha x rays may be used as a nominal current meter to provide an estimate of the characteristic electron distribution created by

University Research Collaborations

Research	Principal Investigator	University
Femtosecond Monochromatic X Rays from Thomson Scattering of Ultrahigh-Power Lasers with High-Brightness Electron Beams	James Rosenzweig	University of California at Los Angeles
Novel Optical Pumping Sources for Coherent Anti-Stokes Raman Microscopy	Denise Krol	University of California at Davis
High-Average-Power, Short-Pulse Laser	Roger Falcone	University of California at Berkeley
Investigations of Energy Transport in Over-Dense Material Initiated by Ultrashort Pulse, High-Energy Laser Pulses	Richard Freeman	University of California at Davis
Synchrotron Radiation from Intense Circularly Polarized Light	Kenneth Wharton	San Jose State University
Development of a Parallelized Three-Dimensional Quasi-Static Particle-in-Cell Code for Studying Short-Pulse Laser Plasma Interactions	Warren Mori	University of California at Los Angeles
Laser Spectroscopy for Evaluation of Transplant Tissue Viability and Early Detection of Rejection	Christoph Troppmann	University of California at Davis
Dense Plasma Characterization Using Transient X-Ray Laser Interferometry	Jorge Rocca	Colorado State University

4 Experimental setup for investigating energy transport in solids irradiated with ultrashort, high-energy laser pulses. Results are consistent with computer modeling, which show lateral as well as forward electron transport.



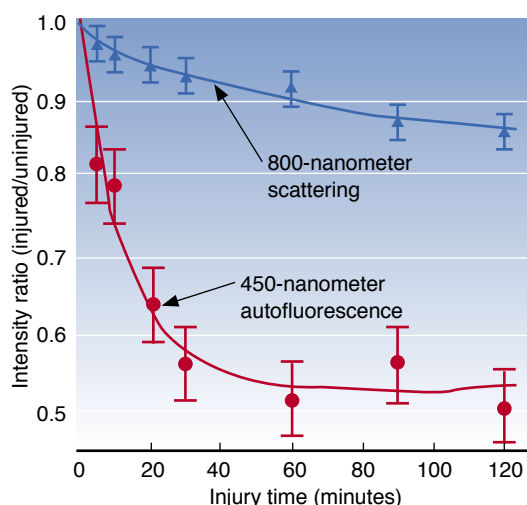
the laser pulse in solid-density matter. The use of ultrashort (sub-picosecond) laser pulses makes it possible to observe emitted x rays before the target disassembles because of hydrodynamic motion, thus allowing us to probe electron transport phenomena in solid-density matter.

In this work, we have observed good agreement between the experimental data for K-alpha x rays and the predictions of a computational model that combined measured laser focal spot data with ponderomotive kinematics (motion resulting from the force acting on electrons because of the alternating current electric field associated with laser light) of the electrons and a Monte Carlo treatment of collisional transport of electrons through matter. Comparison of the experimental data and computational modeling suggests that the transport of relativistic electrons at solid density, while strongly forward directed, is divergent at ~ 45 degrees half angle. We also observed that the diameter of the K-alpha x-ray emitting region was much larger than the laser spot size (11 micrometers), even when the thickness of the aluminum target was extrapolated to zero. Both the experimental data and computational model suggest there is significant lateral (perpendicular to the laser beam) electron transport [*Journal of Quantitative Spectroscopy and Radiative Transfer* **81**, 183 (2003)].

Richard Freeman (freeman@mps.ohio-state.edu)

Laser Spectroscopy for Evaluation of Transplant Tissue Viability and Early Detection of Rejection

Noninvasive evaluation of tissue viability of donor kidneys used for transplantation is an issue that current medical technology is unable to address. The goal of our research was to determine whether optical spectroscopic methods used during hypothermic preservation are capable of measuring the amount of warm ischemia sustained by a kidney before preservation. The hypothesis was that ischemic damage to kidney tissue would give rise to changes in its optical properties that in turn may be used to assess the degree of tissue injury. This project was a collaboration between Livermore and UC Davis and involved researchers and graduate students from the Department of Surgery at the UC Davis Medical Center.



Two optical spectroscopic techniques were explored: (1) autofluorescence of the tissue, which can quantify hypoxia-related fluorophores in the tissue, and (2) near-infrared light-scattering imaging, which can detect cellular and molecular changes in the tissue. The experimental results demonstrated that the autofluorescence intensity of the kidney decreases as a function of time exposed to ischemic injury. Changes were also observed in the near-infrared light-scattering intensities, most probably arising from changes because of injury to and death of the tissue. The lifetimes of the decay profiles shown in Figure 5 are different, indicating that each method provides information on a different mechanism relating to tissue injury associated with alterations in its metabolism and structure. Experiments for in vivo evaluation of this method are in progress.

Christoph Troppmann (christoph.troppmann@ucdmc.ucdavis.edu)

5 Images of the uninjured and injured kidneys from the same rat obtained with tissue autofluorescence at 450 ± 20 nanometers using 335-nanometer light for excitation (**top**) and the injured-to-uninjured ratio of intensity of kidney images (**bottom**) obtained using autofluorescence at 450 nanometers under 355-nanometer excitation (red circles) and cross-polarized, near-infrared light scattering at 800-nanometer illumination (blue triangles).



M Division

MEDICAL PHYSICS AND BIOPHYSICS DIVISION

The Medical Physics and Biophysics Division (known as M Division) aims to advance the biomedical science and technology needed to counter bioterrorism as well as develop better and less costly medical diagnostic devices and therapies. As part of our research, we provide instrumentation to study the biochemistry, physiology, and dynamic structure of living cells. We are also developing new instrumentation and measurement technologies for portable biowarfare-agent detection and monitoring.

Supporting these activities are our core competencies in biosensors; biophotonics; mass spectrometry; micropower radar systems; and infrared, ultrasound, microwave, and x-ray imaging. These same technologies can also be used to diagnose and monitor the spread of infectious diseases, such as influenza, tuberculosis, pneumonia, cholera, and antibiotic-resistant bacteria as well as to screen for the presence of various cancers and monitor their response to therapies. We also have considerable expertise in designing photon-based techniques to activate microtools and visualization systems for intravascular catheter systems. We have computational expertise and simulation codes to study photon transport within, and effects upon, human tissue. Additionally, we have applied the capabilities developed for medical and biodetection research to the needs of the nuclear weapons program by creating new tools for the long-term surveillance of the nation's weapons stockpile.

M Division frequently collaborates with and supports programs throughout Lawrence Livermore, including the Chemical and Biological National Security Program; Biology and Biotechnology Program; Chemistry and Materials Science Directorate; Engineering; Defense and Nuclear Technologies Directorate; Nonproliferation, Arms Control, and International Security Directorate; and Homeland Security Organization.

Shaped Memory Polymer Medical Devices

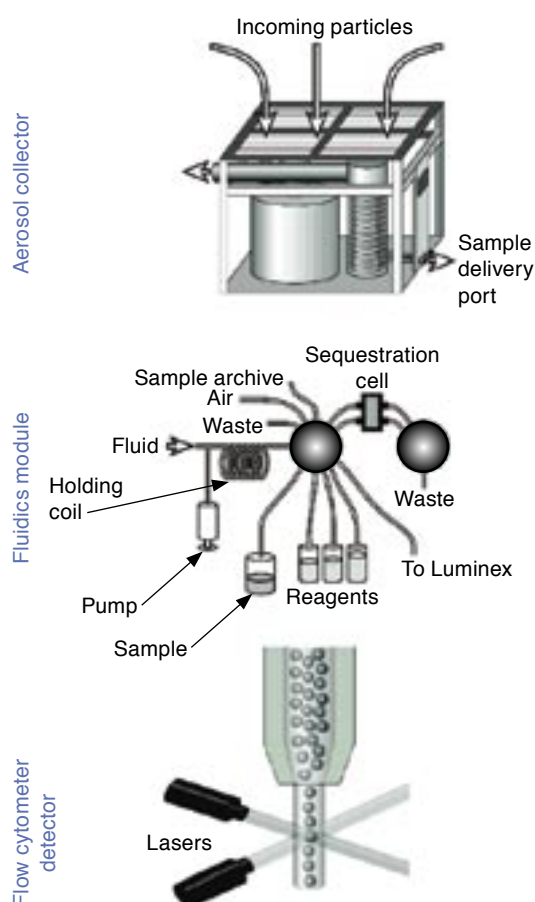
In collaboration with researchers from Chemistry and Materials Science and the University of California at Davis, we have developed a new medical device using shaped memory polymers (SMPs). These polymers can change their shape when heated and then re-form to their original shape on subsequent cooling. This property enables the fabrication of advanced microdevices for medical applications. The new device, a blood clot remover activated by a fiber-coupled laser, has now been demonstrated in prototype form, and is compatible with minimally invasive catheter devices.

Each year, hundreds of thousands of patients suffer an ischemic stroke caused by a clot blocking an artery feeding the brain. Drug therapy is only effective if the patient is treated within three hours of the stroke. According to physicians, SMP-based devices could make a significant difference because it would be possible to treat a patient up to six hours after a stroke.

Operation of the device is as follows. The SMP wire, which is at the end of an optical fiber, is placed into a catheter that is only 0.5 micrometer wide. The bundle is pushed through the artery until it reaches the clot. Then the wire is heated by shining a laser's infrared light down the fiber. The heat changes the wire into either an umbrella or coil shape. This shape change happens in a few seconds. The coil grabs the obstruction from behind, whereas the umbrella can grab the clot from the front. The catheter is then retracted with the clot captured within the umbrella or coil. So far, the research team has used the SMP-based device to spear clots of pig's blood in vitro (i.e., outside the pig's body in an artificial environment). Tests have shown the wire could hold a clot securely against a flow of liquid at more than 10 times the blood pressure normally found in the brain. Animal model testing will continue for about another year.

(Duncan Maitland, maitland1@llnl.gov)

1 The Autonomous Pathogen Detection System is composed of several independent, integrated modules within a rugged, mobile chassis (**top**). The stainless-steel aerosol "stack cap" and cellular communication transmitter extend from the chassis top. Schematic of the aerosol collector (**second from top**). The particle fractionator (four panels on top) screens incoming particles (white arrows), and the virtual impactor (cylinder at lower left) separates particles based on size and is tuned to select particles in the 1- to 10-micrometer range. A wetted wall cyclone (cylinder at lower right) captures particles in fluid; at prescribed intervals, the fluid is dispensed (arrow pointing to the right) to the fluidics module. The sample preparation fluidics module (**second from bottom**) conducts automated immunoassays. Upon completion of the assay, the sample is moved to the detector for analysis. Schematic of sample flow path in the detector (**bottom**). The 100-microliter sample contains several thousand beads, which are embedded with precise ratios of red and infrared fluorescent dyes yielding an array of 100 different bead classes, each class having a unique spectral address. Each optically encoded and fluorescently labeled microbead is interrogated in the flow cytometer using two lasers. A classification laser (635 nanometers) excites the dye molecules inside the beads, and a reporter laser (532 nanometers) excites the fluorescent molecules bound to the bead surfaces. The flow cytometer is capable of reading hundreds of beads per second. After analysis, results are shown on the display panel located on the chassis door.



Microdot Array Sensors

This project aims to develop minimally invasive, optical-fiber-based imaging biosensors for measuring multiple biomarkers, in vivo. Biomarkers are specific biochemicals in the body with particular molecular features useful for measuring the progress of disease or the effects of a treatment.

We have developed an automated contact-based inkjet system for printing multiple microdot array sensors on the polished surfaces of optical fiber bundles. The system uses rigid capillary pins for transporting indicator chemicals to the fiber surface. Each bundle is composed of thousands of individual fibers drawn into a coherent bundle, allowing the transmission of images from one end of the bundle to the other. Each microdot sensor element overlaps several fibers and contains a unique biomarker assay. Because each fiber delivers light that is spatially distinct from its neighbors, it is possible to simultaneously identify each microdot and perform parallel assays by imaging the tip of the fiber bundle.

Microdot array sensors are well suited for measuring biomarkers for infectious diseases, blood-gas levels, and other clinically important parameters. The initial phase of our research has focused on developing pH, oxygen, and enzyme-based biosensors for detecting biomarkers related to stroke and periodontal disease as well as for breast cancer detection.

(Chance Carter, carter45@llnl.gov)

Autonomous Pathogen Detection System

We are part of large, multidisciplinary teams at Lawrence Livermore that are developing new instruments for detecting high-priority pathogens relevant to homeland security. One such team has developed a fully autonomous pathogen detection system (APDS) capable of continuously monitoring the environment for airborne biological threats (Figure 1). The APDS is completely automated, offering continuous aerosol sampling, in-line sample preparation fluidics, multiplexed detection and identification immunoassays, and nucleic-acid-based polymerase-chain-reaction amplification and detection. Continuous, unattended operation has been benchmarked at eight days, at which point only simple refills of the reagents are required. The performance of the fully integrated APDS has

been evaluated in tests inside closed chambers at the Dugway Proving Grounds, where the system was challenged with aerosols containing two live, virulent biological threat agents—*Bacillus anthracis* and *Yersinia pestis* [*Analytical Chemistry* **75**, 5293 (2003)].

The APDS was developed to provide early warning of a bioterrorism incident and can be used at high-profile events for short-term, intensive monitoring or in major public buildings or transportation nodes for long-term surveillance. Individual units can be networked to a single command center so that a small group of technicians can maintain and respond to alarms from any of the deployed sensors. To date, the system has collected and processed more than 10,000 samples in the laboratory and 1500 samples from the field, and additional units are being built for deployment in 2004.

(Mary McBride, mcbride2@llnl.gov)

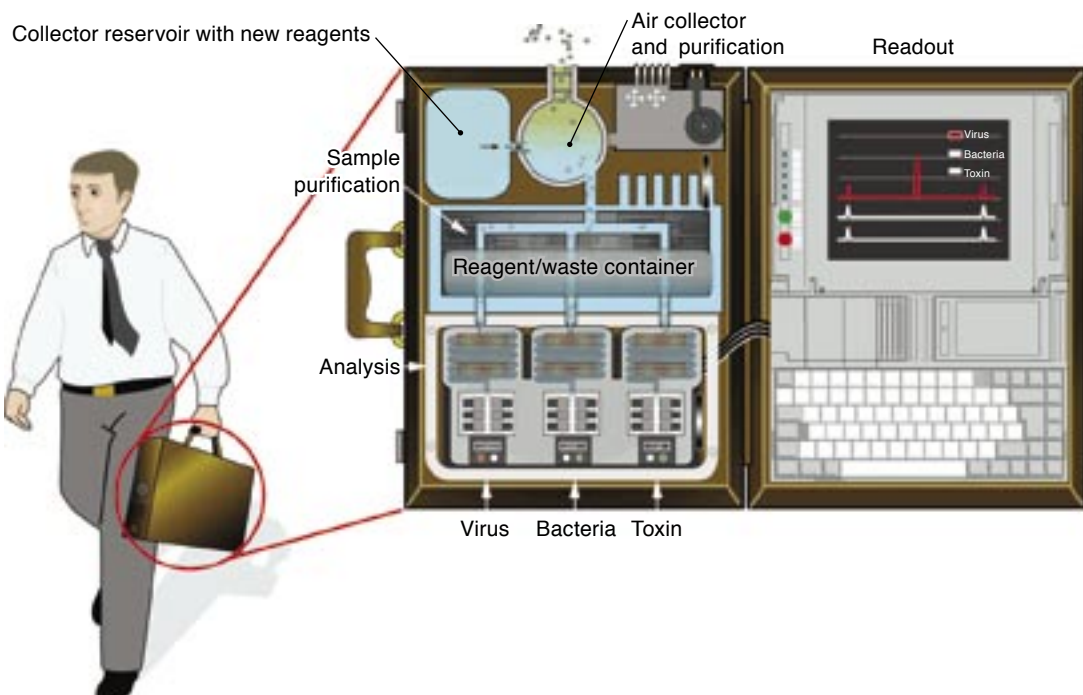
BioBriefcase

In an effort to create a biodetection system smaller than the APDS, Lawrence Livermore and Sandia national laboratories have teamed to develop a portable device, named BioBriefcase. This will be a compact instrument capable of detecting the full spectrum of bioagents including bacteria, viruses, and toxins (Figure 2). When deployed, the system will be used to autonomously monitor the environment for

biological threat agents in short-term situations, including special events, and in major public facilities for long-term surveillance. Intended users of the BioBriefcase include the Secret Service, the Department of Defense, and the Department of Agriculture as well as first responders or law enforcement agencies responsible for protection at major public events.

The BioBriefcase is designed to feature rapid response, multiplex capability, minimal reagent consumption, and decreased cost and size, while maintaining or improving sensitivity and response time compared to currently available technologies. These achievements are made possible through the use of electrophoretic tags for separation and detection of bioagents using capillary electrophoresis, chip-based sample processing modules, and microfluidic sample handling. The device will use three separate and independent analysis tools—a nucleic acid assay, immunoassay, and protein signature. These will provide parallel analysis methods for the detection of bacteria and viruses (nucleic acid assay and immunoassays) and toxins (immunoassays and protein signatures), resulting in multiplex assays with excellent sensitivity and specificity. The team has completed the system design, which uses microfluidics and chip-based modules for sample preparation and analysis. Fabrication of the prototype is under way.

(Anthony Makarewicz, makarewicz1@llnl.gov)



2 Artist's rendering of the BioBriefcase, an autonomous, compact bioagent detector under development by Lawrence Livermore and Sandia national laboratories. The open briefcase displays the control computer and readout (right) and the various detector components (left). The detector consists of the sample collector and reservoir (near the top), the reagent container and sample purifier and separator system (middle), and components of the three parallel analysis systems, one each for viruses, bacteria, and toxins (bottom).

Bioaerosol Mass Spectrometry

We are collaborating with researchers in the Chemistry and Materials Science and Engineering directorates at Lawrence Livermore to develop a technique for rapid analysis of single cells based on single-particle aerosol mass spectrometry. The bioaerosol mass spectrometer (BAMS) analyzes the biochemical composition of single, micrometer-sized particles, such as bacterial cells or spores, that can be directly sampled from air or a suspension. Incoming individual particles are irradiated with a laser pulse that desorbs and ionizes characteristic molecules from the particles. Subsequent time-of-flight mass spectrometric analysis determines the molecular masses of those molecules and reveals characteristic mass-spectral fingerprints that are used to identify the particles. This whole analysis process takes only a fraction of a second per particle. Applications of BAMS include rapid detection and identification of biological warfare agents and “white powder hoax” materials, studies of cell cycles and cell viability, screening of human effluents for pathogens, and possibly, screening of cell samples for cancer.

This started as a Lawrence Livermore Laboratory Directed Research and Development project a few years ago. Initial work demonstrated

that unique mass signatures can be obtained from single bacterial spores with BAMS, and those signatures are very different from many common white powder or hoax materials. The first prototype demonstrated that it could discriminate between some of the species within the genus of *Bacillus*. These results led to significant interest and funding from the Department of Defense for development of a high-throughput bioaerosol detection device based on aerosol mass spectrometry. Another application we will be investigating is the rapid screening of human effluents (such as breath and urine) for pathogens and markers for early diagnosis of diseases and, possibly, screening of plane or ship passengers on international trips.

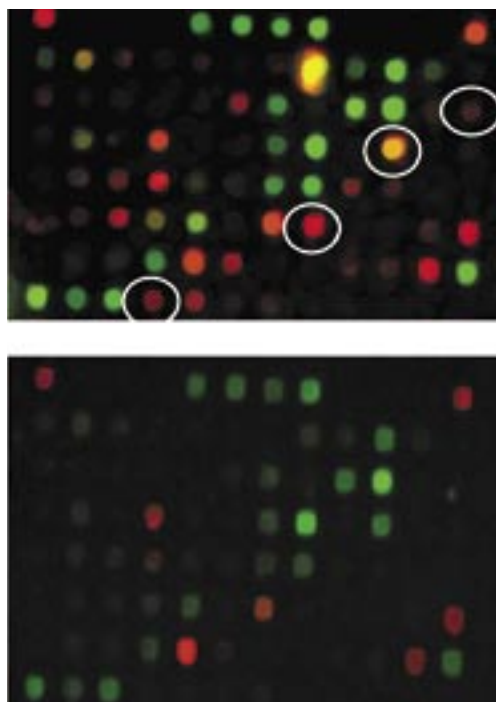
(Matthias Frank, frank1@llnl.gov)

Pathomics Initiative

“Pathomics” is a comprehensive strategy for understanding human response to infectious disease agents, particularly those associated with bioterrorism. Its overall goal is to predict all possible routes of pathogenicity and host response from our understanding of the genes involved, and to have detection systems that will determine if an attack or disease outbreak is beginning prior to people becoming overtly sick. This research is critical to our ability to deal with public health threats from naturally occurring contagious diseases, and importantly from bioterrorism or genetic manipulation. It is a “grand challenge” problem that ultimately will require decades of research.

We are actively involved in the pathomics initiative, along with colleagues from other Lawrence Livermore directorates and research institutions around the nation. The near-term goal is to demonstrate that detection of disease is possible presymptomatically and that molecular signatures can distinguish between pathogen types. The research is initially focusing on a vaccine strain for smallpox and the infectious cowpox virus. We will develop a preliminary type of diagnostic platform and demonstrate its use in public health surveillance. Finally, we will use Lawrence Livermore’s extensive capabilities in informatics and computational modeling to create preliminary models of combined pathogen and host response systems or pathways and show that they can be used to distill common pathogenic effects. Our longer-term vision of

3 Images displaying gene microarray data for blood collected after exposure to a smallpox vaccine (**top**) and normal, control blood (**bottom**). Green dots indicate genes less active in transcribing information from the DNA to the protein-forming system of the cell (down-regulated). Red dots indicate genes that are more active in transcribing information (up-regulated). The circles in the top image identify four of the genes that demonstrate significant differences in the smallpox-infected blood. This comparison illustrates the potential for identifying the presence of infection or disease before the affected individual shows clinical symptoms.



pathomics research is to include many more types of pathogens and much more detailed models of pathogenesis, virulence, and host response and to develop a diagnostic system that could lead to a “bioshield” for the country.

During the first year of the initiative, we have already demonstrated the feasibility of presymptomatically detecting the mild infection caused by smallpox vaccination (Figure 3).
(*William Colston, colston1@llnl.gov*)

Comparison of Immunodiagnostic Methods

Rapid detection and identification of biological warfare agents is vital to initiating appropriate and timely response strategies. We were selected to participate in a Department of Defense–funded study, coordinated by the US Army Medical Research Institute for Infectious Diseases, that compared advanced immunodiagnostic assays for detecting biological warfare agents. Performance evaluation of various immunodiagnostic methods were undertaken to identify the strengths of different technologies.

Our study involved developing and validating a multiplex assay using Luminex technology for detecting Venezuelan encephalitis virus, staphylococcal enterotoxin B, and *Yersinia pestis* F1 antigen. We developed a fluorescent, microsphere-array multiplex assay for detecting the agents’ antigens. Immunoreagents used in the study were provided by the US Army Medical Research Institute for Infectious Diseases as part of the comparative performance evaluations. Detection of the antigens was tested in three sample matrices—buffer, serum, and urine. A number of internal controls were incorporated to enhance confidence in the assay performance, and once the assay optimization was completed, a blind study was conducted using more than 1350 coded samples.

The fluorescent microsphere multiplex assay had very good detection limits for simultaneous detection of the three test agents, and it had excellent intra- and inter-assay reproducibility. Inclusion of internal controls in every test sample significantly increases the confidence in the assay result by allowing errors in assay performance to be easily monitored. The multiplex assay developed in this study has great potential for rapid detection and identification of biological warfare agents—it is highly scalable, with the potential for up to 100 targets to be

simultaneously detected using the same assay format. When sufficiently multiplexed, this assay also has the potential for significant time and cost savings.

(*Venkat Venkateswaran, venkateswaran2@llnl.gov*)

Sentinel Chicken Surveillance

West Nile virus is a mosquito-borne disease in humans, horses, and birds. Since it was first detected in New York in 1999, more than 4000 cases have been detected in 44 states, including California. Sentinel chickens become infected, without clinical illness, by mosquitoes carrying the West Nile and other viruses including St. Louis encephalitis virus and western equine encephalitis virus. Sentinel chicken surveillance has proved useful for detecting the West Nile virus in Florida and other states.

We designed and developed a fluorescent microsphere multiplex immunoassay for serological antibody testing in chickens. This project was conducted in collaboration with Viral and Rickettsial Disease Laboratory, California State Department of Health Services, in Richmond. The three virus antigens and control antigens were coated on separate sets of optically encoded microspheres. The multiplex assay was optimized for detection of antibodies in blood samples. This assay was performed on eluates from chicken blood collected on filter papers, and chicken serum. The assay performance was compared with enzyme immunoassay and fluorescent antibody test for the same antibodies. Our fluorescent microsphere multiplex immunoassay was useful in simultaneously detecting antibodies to all three of the viruses in these tests. We found that our assay results were comparable to the corresponding enzyme immunoassay results. Incorporating internal controls in the multiplex assay considerably reduced the potential false negative and false positive results. Our assay results were also comparable to the conventional, indirect fluorescent antibody results.

This project has demonstrated the usefulness of multiplex antibody detection for sentinel chicken surveillance programs. Because this detection scheme is amenable to automated, high-throughput application, it has great potential for large-scale serological testing of chickens for vector-borne viral exposures.

(*Thomas Bates, bates13@llnl.gov*)

Biological Assay Development

A critical component for many of the biodetection systems currently under development is the bioassay used in the detection process. We are exploring a range of detection and identification technologies to develop assays that are rapid, sensitive, specific, and cost-effective. We have successfully demonstrated highly multiplexed, bead-based antibody assays (Figure 4) that are capable of simultaneously detecting 15 different biological agents from a single sample [*Analytical Chemistry* **75**, 1924 (2003)].

This immunoassay development has been directed at detecting biological threat agents (e.g., the National Institute of Allergy and Infectious Diseases Category A, B, and C Priority Pathogens). The assays have been extensively tested against live virulent agents, large numbers of strains and strain preparations, and panels of near-neighbors. Assay performance has been evaluated in a variety of complex sample matrices including serum, blood, and soil. The multiplexed immunoassays are

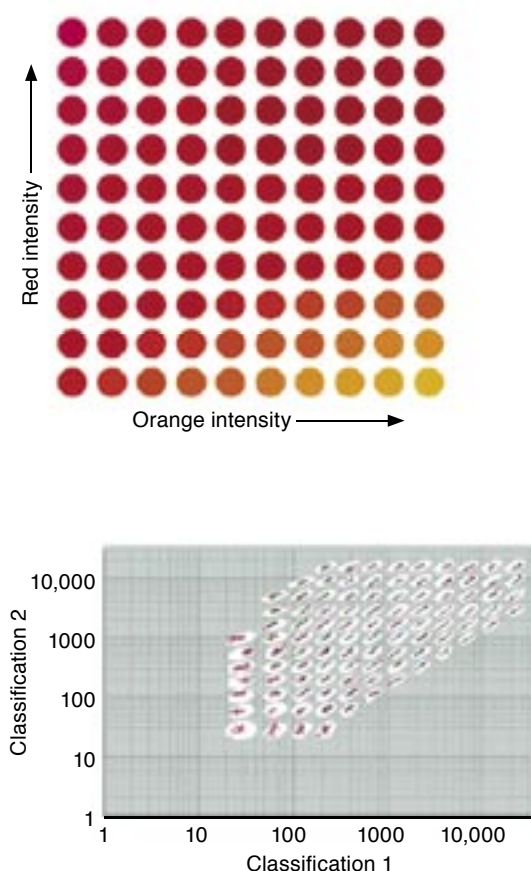
undergoing validation, with plans to disseminate the assays to the laboratory response network and make them commercially available.

Similarly, we have developed nucleic-acid (DNA) assays using the TaqMan-based polymerase chain reaction system and extensively tested them for detection of biological threat agents. Polymerase chain reaction assays have been tested on hundreds of samples obtained in the field, and the required reagents have been subjected to a wide range of storage conditions to assess their robustness.

The next phase of this research will focus on developing similar assays for clinically relevant pathogens (e.g., influenza, staphylococcus, and tuberculosis) that can be used in public health and hospital-based laboratories. We are teaming with industrial partners, academia, and government to develop a small, affordable diagnostic platform that can be used in hospitals and will also be well suited for applications in resource-poor, underdeveloped countries.

(Mary McBride, mcbride2@llnl.gov)

4 This liquid array-based sensor is designed for rapid, sensitive, specific, and simultaneous detection of multiple biological agents. A 100-plex Luminex liquid array is generated by injecting varying amounts of both red and infrared dyes into polystyrene microspheres (**top left**). Each optically encoded bead has a unique spectral address. Beads are coated with capture antibodies specific for target antigens (**top right**). After incubation with the antigens, detector antibodies are added, followed by addition of the fluorescent reporter. The beads are analyzed in the flow cytometer, using two lasers to interrogate one bead at a time (**bottom right**). The red laser identifies the bead type. The green laser quantifies the assay on the bead surfaces through fluorescence, whose signal is a function of antigen concentration. Dot plot of 100-plex bead analysis (**bottom left**). The white circular regions represent the 100 beads; colored dots in each region represent detection events for the corresponding bead.



Biophotonics and Genomes to Life

We are collaborating with researchers in the Chemistry and Materials Science Directorate to develop novel optical tools for detecting specifically tagged individual proteins and complexes of proteins, which form the machinery of life [*Applied Spectroscopy* **57**, 868 (2003)]. Noble metal (e.g., gold) nanoparticles between 40 and 100 nanometers (nm) are used as tags because they have been shown to efficiently scatter portions of the optical spectrum when illuminated with white light. The wavelength of light scattered depends on particle diameter and is determined by the surface plasmon resonance of these particles, a mode whereby all conduction electrons oscillate synchronously.

With modern optical detection tools, such as intensified charge-coupled-device cameras, we can observe individual nanoparticles with very high spatial and temporal resolution. When the nanoparticle tags are attached to motor proteins or molecular machines (molecules that are able to convert chemical energy, from nucleotide hydrolysis, into the mechanical force necessary to power cell movement), the scattered light from them reports the current position of the proteins as they process DNA. These positions can be accurately monitored with our optical detection system to within ~10-nm precision and then turned into a vector-field description of the molecular motion. This results in our ability to measure, for example, sequence-specific processivity rates for protein machines that are otherwise hardly accessible, providing new insights into the fundamental processes of life.

(Steve Lane, lane12@llnl.gov)

Collaborations with University of California at Davis

We collaborate extensively with researchers at the University of California Davis Cancer Center and the Center for Biophotonics Science and Technology. In one of the projects, we are working with two physicians in the Pediatric Oncology Department to develop a microscope that can optically trap individual cells and spectroscopically analyze their vibrational signature. Ideally, such a system would be able to identify individual cancer cells in liquids such as blood. Molecular vibrations within biomolecules can scatter light and produce well-defined, narrow spectral peaks as the signature of the scattering process. Analysis of the (Raman) scattered light spectrum permits us to determine the frequency

of molecular vibration, which is unique depending on the atoms involved. Thus, the vibrational spectra allow for compositional analysis of biomolecules.

Our research has focused on identifying distinctive differences between tumorigenic and nontumorigenic cells. Tumorigenic cells typically have much larger nuclei and their metabolism is significantly different from regular cells, which should result in distinct changes in their vibrational spectrum. An optical detection system based on molecular vibrational signatures would have a number of clinical applications, such as early cancer detection or monitoring the response to treatment.

(Dennis Matthews, matthews1@llnl.gov)

Diagnostics of Nuclear Weapons Components

Diagnostic methods and technology developed for medical applications also offer improved capabilities for inspection and surveillance of nuclear weapons components required under the Stockpile Stewardship Program. We are actively involved in efforts to provide such capabilities to the Department of Energy (DOE) nuclear weapons complex. Recently, we developed a sub-millimeter-diameter fiber-optic endoscopy tool and used it to evaluate multiple nuclear weapons components. The endoscope optics were designed to collect undistorted images, permitting accurate metrology of the weapons components. In the future, we have plans to add a spectroscopic imaging capability to the endoscope to evaluate material properties and identify possible contaminants, through the use of spatially resolved fluorescence and Raman spectroscopy.

Medical computed tomography scanner technology offers the potential for producing high-resolution, three-dimensional x-ray images of nuclear weapons components. We participated in the development of a prototype x-ray tomography system for the DOE weapons complex. The prototype, built and tested at Livermore, was used to produce the first three-dimensional images of nuclear weapons components during nondestructive evaluation of stockpiled warheads. An operational system based on this prototype is now being installed at DOE's Pantex facility for long-term surveillance. An advanced x-ray tomography system, with significantly higher spatial resolution, is under development.

(Jim Trebes, trebes1@llnl.gov)



Fusion Energy

FUSION ENERGY PROGRAM

The Fusion Energy Program develops, in collaboration with national and international partners, the science and technology required to pursue fusion as a long-term energy source. We have significant capabilities in large-scale experimental operations, diagnostics development, advanced plasma theory, and large-scale simulation. Our fusion research covers both magnetic fusion energy (MFE) and inertial fusion energy (IFE), and much of this research is supported by the Department of Energy's Office of Fusion Energy Sciences.

Currently, we operate two major experiments at Lawrence Livermore—the Spheromak is used to explore an alternative confinement concept for MFE, and the Source Test Stand is used to investigate ion sources for heavy-ion-driven IFE. Collaborations with other fusion institutions include major partnering roles in experiments on the DIII-D tokamak at General Atomics in San Diego and in the Heavy Ion Fusion Virtual National Laboratory, which is a partnership involving Lawrence Livermore, Lawrence Berkeley, and Princeton Plasma Physics laboratories. We also participate in National Nuclear Security Administration-funded research on inertial confinement fusion and laser-driven IFE.

Two years ago, we began a realignment of MFE-related research activities to focus on two broad technical areas:

- Tokamak edge physics and its relationship with physics of the plasma core.
- Physics of spheromaks and related configurations.

Highlights of recent research in these areas are described below.

The Fusion Energy Program also houses the Beam Research Program, which is developing advanced technology for the Dual Axis Radiographic Hydrodynamics Test (DARHT)—a major stockpile stewardship facility at Los Alamos National Laboratory in New Mexico—and compact particle accelerators for radiography and other applications.

Magnetic Fusion Energy Theory

The Magnetic Fusion Energy Theory Group provides theory and modeling support for ongoing experimental programs on the DIII-D tokamak and the Sustained Spheromak Physics Experiment (SSPX) at Livermore. We also carry out complementary research in turbulence and integrated modeling of core plasmas. A major development was the October 2003 approval of a strategic initiative, funded by Livermore's Laboratory Directed Research and Development Program, to develop an integrated, kinetic simulation code for modeling turbulent transport in the boundary region of tokamak plasmas. An expected outcome of this three-year initiative, which involves collaboration with Livermore's Computation and Chemistry and Materials Science directorates, is to be able to predict from first principles the height of the edge transport barrier that determines the overall fusion power output of next-generation tokamak reactors.

Our research on tokamak edge physics and its interaction with the plasma core has focused on three key issues concerning successful tokamak operation with good core confinement and acceptable power and particle-handling capabilities:

- The edge transport barrier with the ensuing H-mode pedestal formation from plasma pressure.
- The role of turbulence, fueling, and impurities in the edge plasma.
- Distribution of particle and heat flux to divertors and chamber walls.

We have used the Livermore-developed, BOUT three-dimensional edge turbulence code—arguably the best of its class in the world—to improve substantially our understanding of all three of these issues in the past year, and we have demonstrated increasing ability to compare with experimental data obtained at major US MFE facilities [*Physics of Plasmas* **10**, 1773 (2003)]. In the area of core physics, we studied the role of kinetic electron effects (e.g., trapped electrons), electromagnetic coupling to shear-Alfvén waves

(i.e., waves with small perpendicular scales), collisions and noncircular flux surfaces in influencing ion-temperature-gradient turbulence and concomitant transport with self-consistent shear flows, and internal transport barriers. As part of this work, we have collaborated with colleagues at the University of Colorado and University of California at Los Angeles on the SUMMIT code framework to extend the capabilities of our gyrokinetics code and the range of physics applications we undertake.

For integrated modeling of MFE plasmas, we use the UEDGE two-dimensional transport code for the edge region, and the CORSICA code for the core region. UEDGE is the primary edge-transport code in the US. While CORSICA is one of several integrated modeling codes, it has a number of unique features that make it an essential tool for supporting experimental efforts on DIII-D and SSPX.

The second major thrust of our theory and modeling effort is the physics of spheromaks and related self-organized plasma configurations, such as reversed-field pinches and magnetized-target fusion. In this research, we are working closely with the ongoing experimental program at SSPX in Livermore. To interpret the results of current experiments and to guide future ones, we have identified four key questions:

- Is there a theory recipe for a sustained spheromak with good flux surfaces?

- Is the energy confinement adequate to yield an interesting fusion concept?
- How do spheromak plasmas interact with surrounding structures?
- Are there interesting alternatives to a steadily driven spheromak?

During the past year, we used the NIMROD code to perform parameter and scaling studies of formation and decay of spheromak plasmas [*Nuclear Fusion* **43**, 1120 (2003)]. With NIMROD, we simulated single- and double-pulse scenarios for comparison with results obtained at SSPX. These simulations demonstrated a growing magnetic field and larger closed flux volumes (Figure 1). An analytical study of the stability of a screw pinch, a model for the spheromak central column, showed that growth rates are reduced by finite-length effects and by the introduction of a partial, central plasma column. We have reformulated the equilibrium reconstruction problem in axisymmetric geometry so that we can determine the parallel current profile entirely from core plasma electron-temperature measurements. In addition, we have used the CORSICA code to simulate equilibrium reconstruction, Ohm's law, and energy transport in plasmas created by SSPX.

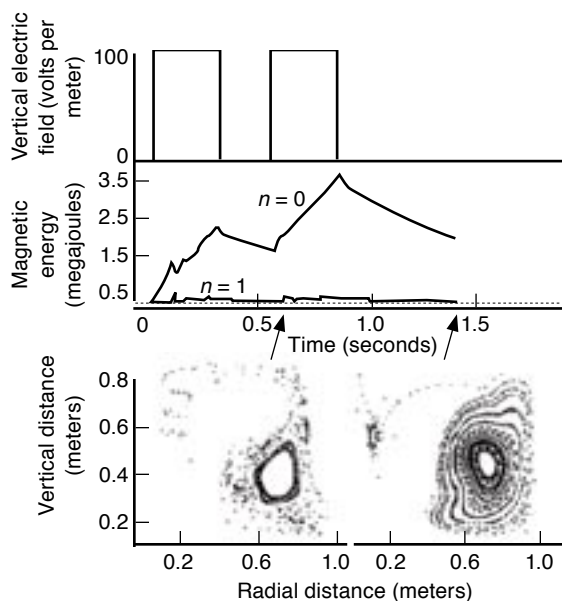
Ron Cohen (cohen2@llnl.gov)

Research at DIII-D

The overall mission of the Department of Energy's research program at the DIII-D facility at General Atomics in San Diego is "to establish the scientific basis for the optimization of the tokamak approach to fusion energy production." Our collaboration on DIII-D involves two areas: advanced tokamak physics and divertor physics, where we lead or contribute to the whole cycle of research; and experimental planning, diagnostic development, execution of experiments, and detailed analysis.

We have focused on measurement and modeling of the current profile in advanced tokamak plasmas. The profile and its importance in determining the magnetohydrodynamic stability of the plasma in a high magnetic field are at the heart of research at DIII-D. We played a key role in developing the motional Stark effect (MSE) diagnostic. We created a new, in situ calibration technique, with a goal of 0.1-degree accuracy in magnetic-field pitch angle measurements. This involved installing precision

1 Results from NIMROD simulation showing growth of magnetic energy and volume of good flux surfaces in a spheromak plasma generated with two pulses. Timing of the pulse sequence (**top**) and time evolution of the magnetic energy in two modes (**middle**). Contours of the flux surfaces (**bottom**) after the two pulses, at 0.57 (left) and 1.4 seconds (right).



polarizers in the DIII-D vessel and measuring MSE signals with all of the DIII-D magnetic-field coils energized (Figure 2). A recently installed new “digital lock-in” data acquisition system has enabled measurements of localized magnetic field perturbations with high time resolution [Review of Scientific Instruments **75**, 2995 (2004)].

The goal of our divertor research is to develop a model of the scrapeoff layer and divertor plasmas and benchmark the model with experimental data. Modeling and previous measurements have always indicated that most of the recycling and fueling for the core plasma comes from the divertor. We now have direct experimental measurements of the plasma core near the midplane to verify this result. We invert charge-coupled device camera images of D_α emission resulting from ionization of neutral deuterium atoms by the plasma to compare the ionization source in the core with that in the divertor, which is more than 100 times greater. We can reproduce the salient features of these data with the UEDGE code. Our analysis of the simulation results shows that the core tokamak plasma is fueled mainly by neutral atoms “leaking” through the thin edge plasma from the divertor.

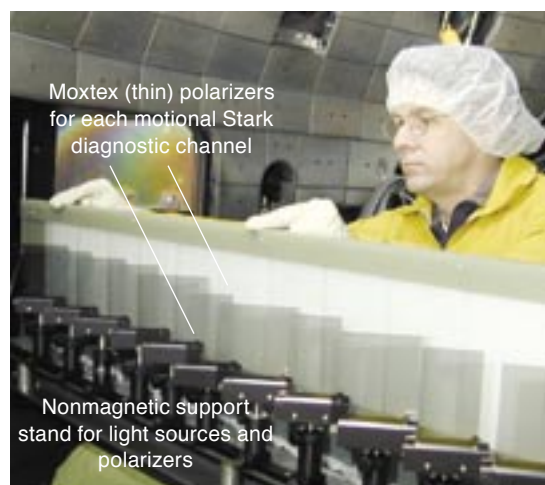
We also used D_α emission measurements, in conjunction with UEDGE simulations, to investigate E-cross-B drift—plasma drifts in the crossed magnetic and electric fields—an

important quantity not previously measured. Shown in Figure 3 are two cases where the drift direction was changed by reversing the direction of the toroidal magnetic field. The predominant region of emission changes from the inner divertor strike point (top figure) to the other divertor strike point (bottom figure) when the direction of the drift is changed.

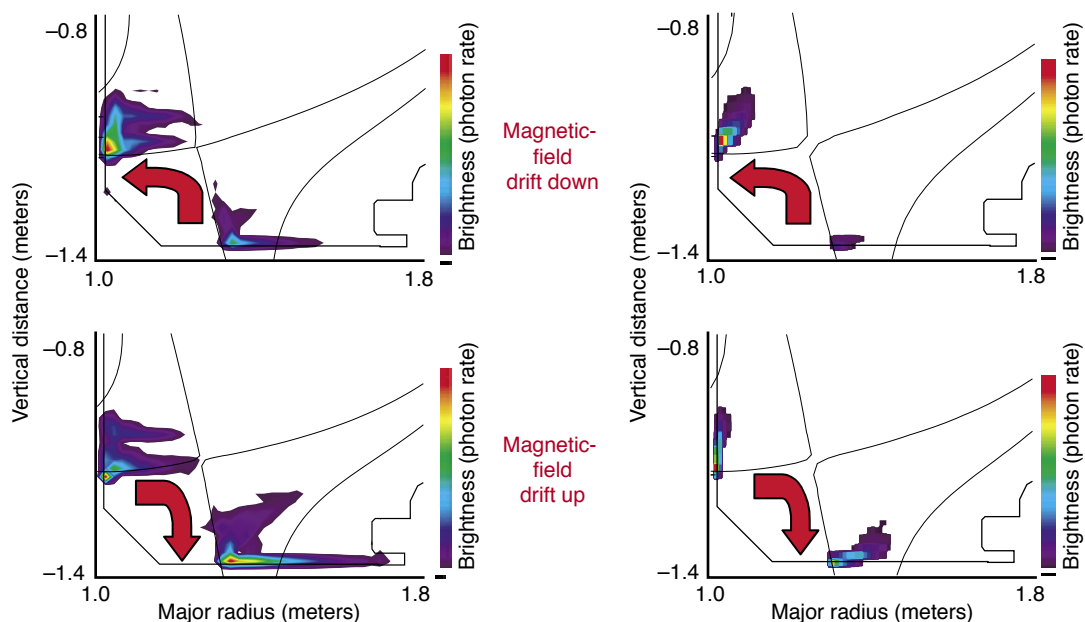
Steve Allen (allen18@llnl.gov)

Spheromak Experiments

The spatial distribution of the electrical current and magnetic field inside the coaxial source sustaining the spheromak plasma are



2 In situ setup of the calibration system for the motional Stark effect diagnostic at DIII-D. Precision polarizers mounted inside the DIII-D vessel during testing provide signals for calibration.

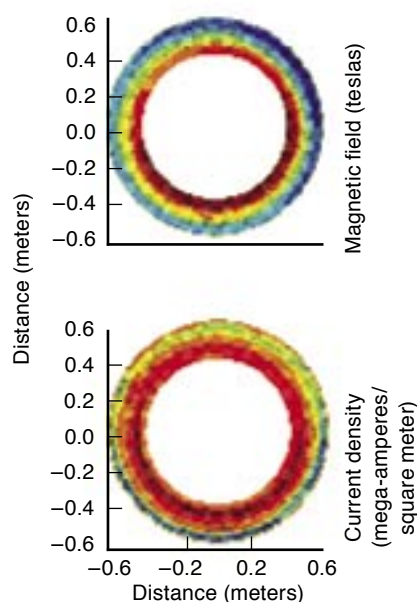


3 Spatial distribution of D_α radiation for two cases of the toroidal magnetic field. Measurements (**left**) and UEDGE modeling (**right**) show that the predominant region of D_α emission changes from the inner divertor strike point (**top**) to the other divertor strike point (**bottom**) when the direction of the magnetic field is reversed (red arrows). This shows the importance of the direction of the E-cross-B drift in the divertor region.

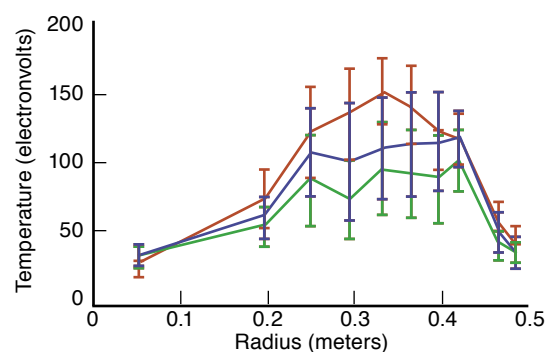
key factors governing the energy efficiency of a spheromak that uses coaxial gun injectors. We have completed the first systematic study of these distributions in the SSPX at Livermore using internal magnetic probes.

Our measurement shows that during the key formation phase, current distribution is not uniform around the coaxial source, counter to the accepted model for such sources. Figure 4 shows a snapshot of the magnetic field and axial current distribution inside the SSPX coaxial source at a single axial cut (the axis of the injector is out of the page). The two-dimensional contour maps show a clear asymmetry (color variations within individual bands), which temporal measurements show to be rotating around the coaxial injector at a frequency of ~20 kilohertz. Interestingly, the spatially integrated field and current do match

4 Contour maps of the magnetic field (top) and current density (bottom) showing the spatial distributions, in a single plane perpendicular to the coaxial injector, inside the Sustained Spheromak Physics Experiment coaxial source, as sampled by a magnetic probe array assuming a rigid-rotor $n=1$ model. The magnetic field ranges from 0.14 (maroon) to 0.01 (light green) to -0.15 (violet) tesla. Current density ranges from 1.6 (maroon) to 0 (yellow) to -5 (violet) mega-amperes per square meter.



5 Measured electron temperature profiles for three cases of the perturbing magnet coil current. Positive coil current corresponds to the magnetic field axis toward the center of the spheromak. Red line is 800 ampere profile, blue line is 0 amperes, and green line is -800 amperes.



standard theoretical models, even though local values can vary as much as a factor of two or more near the injector. The measured variations in the coaxial region may help explain the frequency and direction of rotation of magnetohydrodynamic modes observed in the spheromak plasma produced by the injector. This research [*Physical Review Letters* **90**, 095001 (2003)] formed part of the PhD thesis of a graduate student from the University of Washington.

In multipulse operation of the SSPX, we have shown that the field energy of the spheromak can be increased in a stepwise manner. By controlling the inductive and resistive processes that occur in the plasma, we were able to optimize the energy coupling. Results from the experiment for which the current source was pulsed twice show a stepwise increase of the stored energy from 18 to 32 kilojoules. By this means, we have achieved the strongest magnetic fields in SSPX (0.7 tesla at the geometric axis) and exceeded an important scaling of magnetic field with current.

We have also explored the effects of non-axisymmetric perturbations on plasma confinement in spheromaks at SSPX. A copper coil set was installed with the magnetic axis directed toward the center and along the midplane of the SSPX. We performed experiments to measure the effect of external magnets on SSPX operation. Unexpectedly, confinement was improved, as reflected by the increased measured electron temperature (Figure 5). Reversing the direction of the perturbation field gave poorer confinement and lower temperature.

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Collaboration with Princeton Plasma Physics Laboratory

We have continued our collaborations with the Princeton Plasma Physics Laboratory on the National Compact Stellarator Experiment (NCSX) and the National Spherical Torus Experiment (NSTX), both at Princeton. Here, we highlight our contributions to the NSTX program, which has focused on understanding the boundary plasma region [*Nuclear Fusion* **43**, 1653 (2003)].

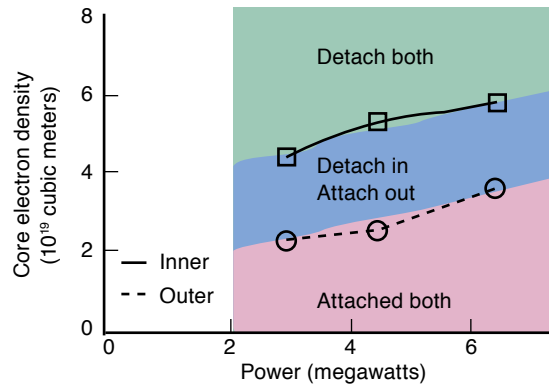
We used the UEDGE code to study expected behavior of the NSTX boundary plasma as a function of heating. We simulated double null configurations, to assess the up/down asymmetry of divertor heat and particle loads, and specific single null discharges, to compare the simulation

with measurements. One issue identified in this effort has been the inability to determine the location of the separatrix, which marks a boundary between two plasma regions with different properties, because of the limited spatial resolution of the electron density and temperature profile diagnostics at NSTX. The uncertainty in separatrix position then leads to a rather large uncertainty in the anomalous radial transport coefficients used in the UEDGE simulations. These difficulties continue to be the focus of our simulations of the boundary plasma.

One objective of NSTX is to determine the boundaries for detached plasma operation. In diverted tokamaks, the divertor plasma detaches when the upstream density is high enough, or heating power is low enough. Detached operation is characterized by a significant reduction in divertor heating power and hence is highly desirable because less electrical power is required. We completed a series of UEDGE simulations in which the upstream density and the heating power were varied to determine the boundaries for detachment of the inner and outer divertor plasmas. We found that both plasmas will be detached for core electron densities greater than 4 to 6×10^{19} cubic meters at heating powers between 3 and 6 megawatts (Figure 6). The results will be used to guide future NSTX experiments.

To understand the turbulence of the boundary plasma, we performed simulations with the BOUT three-dimensional turbulence code using typical experimental parameters for NSTX. We modeled the boundary-plasma turbulence in a realistic divertor geometry using various assumed edge profiles to study the sensitivity to plasma vorticity, density, electron and ion temperature, and parallel momentum. We found that the resistive ballooning mode plays a crucial role in the boundary plasma. The x-point geometry affects the poloidal mode structures and the drift-Alfvén mode becomes robustly unstable because of low magnetic field.

Filamentlike structures were observed both in the simulations and gas-puff imaging measurements. In the direction parallel to the magnetic field, the correlation length is very long (~ 10 meters), while perpendicular to the magnetic field, the length is only a few centimeters. The typical correlation times are ~ 15 to 30 microseconds at the midplane, which is in agreement with measurements. The frequency spectra of the midplane fluctuating



6 The detachment boundaries of the National Spherical Torus Experiment (NSTX) divertor plasmas predicted by UEDGE code simulations, as a function of core electron density and heating power. The simulations began with an NSTX H-mode plasma.

density from gas-puff imaging measurements and BOUT simulations in L-mode show reasonable agreement. Images of edge turbulence show large-scale, transient, and coherent structures (localized in time and in space) convecting upward through the observation domain at several kilometers per second and reversing outside the separatrix.

In 2004, we will shift the emphasis of our NSTX efforts to experimental research, to obtain additional boundary plasma data needed to benchmark numerical simulations done with UEDGE and BOUT codes.

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Heavy-Ion Fusion

Ion beams produced by induction accelerators have characteristics that make them attractive as a driver for IFE. In addition, such a driver offers a unique way of heating matter to high energy densities. The key technical challenge for IFE is to meet the target focusing requirements at a reasonable cost. Development of these heavy ion beams is the mission of the Virtual National Laboratory that includes scientists from Lawrence Livermore, Lawrence Berkeley, and Princeton Plasma Physics laboratories. Ongoing experiments in intense-beam accelerator physics include the source test stand at Livermore exploring advanced ion sources; the high-current experiment at Berkeley investigating ion-beam emittance growth, halo formation, and electron-cloud interactions; and the neutralized transport experiment at Berkeley studying the focusing of ion beams in the presence of a neutralizing plasma. These experiments lay the groundwork for an integrated beam experiment that has been identified by the Department of Energy Office

of Science Strategic Plan as the essential next step in the heavy-ion-beam IFE program. Our research efforts in 2003 focused on experiments and simulation of the merging-beamlet ion injector and beam-gas interactions. In addition, we have advanced the theory underlying ion-beam simulations.

We used the WARP particle-in-cell (PIC) code to simulate an ion injector, which consists of merging beamlets (small-diameter beams) of ions, and found that a dense beam-phase space is attainable with this concept. Our results suggest that an alternate ion source configuration, probably more attractive than the traditional large-diameter source, is to merge a large number of high-current-density beamlets to form a high-brightness beam [*Physical Review*

7 The STS-500 ion source injector test stand at Livermore.



Special Topics—Accelerators and Beams **6**, 014202 (2003)]. We also performed experiments on multi-beamlet dynamics at full-voltage gradient in the first few sections of an Einzel-lens injector column mounted on the ion source test stand at Livermore (Figure 7). An array of 61 beamlets was extracted from a radio-frequency-driven argon plasma source. We were able to operate the source with good gas efficiency, and the current density was found to increase with radio-frequency power as long as there was sufficient extraction voltage. At 80-kilovolt extraction voltage, we obtained an ion current of 4.9 milliamperes per beamlet, corresponding to a total current density of 100 milliamperes per square centimeter.

Electron trapping in the potential of multi-kilovolt ion beams, leading to partial neutralization and possible loss in beam control, is a concern in magnetic focusing systems. “Halo” ions impacting the wall can also generate secondary electrons, ions, and atoms. Desorbed gas increases beam-gas interactions that can produce additional electrons within the beam potential. We performed new measurements with the gas and electron source diagnostic on the high-current beam at Berkeley. These experiments indicate that electron and neutral atom yields resulting from 1-megaelectronvolt, singly charged potassium ions incident on roughened surfaces are independent of angle and substantially smaller than those resulting from nearly grazing-incident impacts on smooth surfaces. This finding suggests a possible inexpensive mitigation of problems caused by secondary particle yields in high-current ion accelerators, based on surface roughness. In 2004, we will perform similar experiments at the Livermore source test stand to explore these effects at lower beam energies (60 to 500 kiloelectronvolts).

We have made considerable progress developing a comprehensive set of models for electron-cloud and gas effects in high-current ion accelerators. In a series of linked simulations, we generated a population of secondary electrons from initial ion impacts on walls using an experimentally derived prescription and then tracked the secondary electrons to obtain an electron density profile. We investigated ion-beam dynamics using a variety of electron distributions to determine thresholds for beam degradation and discovered that the thresholds are significantly

affected by resonance of the electron distribution with normal modes of the ion beam.

We continue to advance the theory and computational methodology for studying ion-beam dynamics. For the first time, we demonstrated a capability to launch simulations using a four-dimensional, initial beam-particle distribution derived from experimental measurements to facilitate comparison between experiment and simulation [*Laser and Particle Beams* **21**, 17 (2003)]. We determined the stable propagating regimes (in terms of focusing strength and space-charge parameters) of beams in periodic focusing lattices, in which the beam envelope can, under some circumstances, resonate with the lattice. We also completed a conceptual study of an integrated beam experiment that would test beam manipulations needed for heavy-ion fusion drivers [*Laser and Particle Beams* **21**, 553 (2003)]. We investigated neutralized ballistic focusing of heavy ion beams, including the effects of photoionization of the ion beam and chamber plasma during target heating. We also developed a method for concentrating grid resolution where it is most needed (known as adaptive mesh refinement) in our PIC simulations and incorporated it into the WARP code [*Physics of Plasmas* **11**, 2928 (2004)].

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Heavy-Ion Fusion Target Design and Simulations

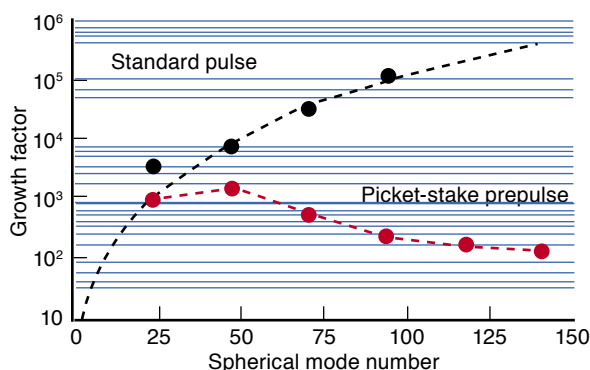
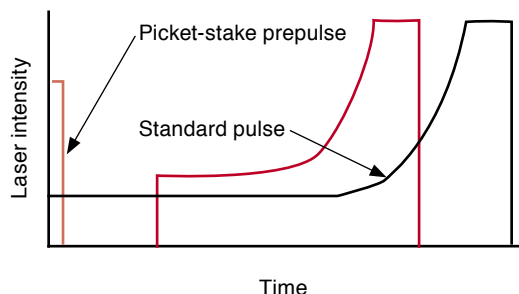
Our fusion target design and simulation research has focused on three areas: three-dimensional simulations of hydrodynamic instabilities during implosions, design of a high-yield capsule that minimizes asymmetries

in spherical implosions, and design of targets directly driven by high-energy lasers.

We have begun three-dimensional simulations of IFE capsules. Such simulations are on the edge of current computing capability—the only other group pursuing this challenge is in Japan. A key physics issue affecting the performance of fusion targets is hydrodynamic instabilities that develop during implosion. These instabilities are seeded by perturbations or imperfections on the surface of spherical targets, which result from fabrication. A specific goal of target design is to establish permissible tolerances for surface roughness.

We have used the HYDRA code to simulate in three dimensions the instabilities associated with targets intended for the National Ignition Facility and found that the earlier two-dimensional simulations overestimated these tolerances by as much as 40%. To determine whether the new stricter requirements also apply to IFE capsules, we performed two- and three-dimensional calculations of single-mode instability with HYDRA. Preliminary results indicate that the instability grows faster in three dimensions than in two dimensions. We are currently examining computational techniques to ensure that the three-dimensional simulations of multimode instabilities are free of artificial growth induced by numerical problems.

Previous design of the heavy-ion hybrid target successfully used a shim layer to correct a P_4 asymmetry (described by the fourth-order Legendre function) during implosion. However, detailed calculations of the capsule indicated that the edge of the shim caused short wavelength perturbations to be excited. To address this problem, we developed an alternate design that removes the edge of the shim and instead covers



8 Inclusion of a “picket-stake” prepulse in the driver laser pulse can significantly reduce growth of the Rayleigh-Taylor instability during target implosion. The temporal profile of the driver laser (**left**), and the calculated growth factors of the various spherical modes (**right**), both with and without the prepulse.

the entire surface of the capsule with a gold layer of varying thickness. This design appeared to work and may allow the shim layer to sit right on the capsule surface. In collaboration with Sandia National Laboratories, we have designed an experiment to test shims in the double-ended Z-pinch hohlraum on the Z-pulse power machine at Sandia. This experiment will be fielded following measurements of the P_2 and P_4 asymmetries of the double-ended Z-pinch hohlraum itself.

We also studied the design and performance of laser-driven, direct-drive targets for IFE. We significantly improved the stability of these targets by using a laser pulse shape that includes a large prepulse before the main pulse. This “picket-stake” prepulse substantially reduces growth of Rayleigh-Taylor instability (as evidenced by growth of spherical modes) because of higher laser ablation velocities. As shown in Figure 8, at spherical mode numbers around 100, their growth factors have been reduced from ~100,000 to only ~300, which are comparable to those seen for targets indirectly driven by heavy-ion beams.

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Heavy-Ion Fusion Power Plant Study

Significant progress has been made in recent years in all aspects of heavy-ion inertial fusion including target design, driver optimizations, driver/chamber interface, and many aspects of thick liquid-wall chambers, which have the promise of enabling first walls to survive for the life of the power plant. We completed a study of an integrated power-plant design that is self-consistent and based on current best understanding of target and accelerator physics, beam propagation and focusing, final focus magnet design and shielding, and chamber dynamics.

The design parameters were selected conservatively to allow each design part to meet its functional requirements in a robust manner, with the key goal of assessing scientific and technical viability of heavy-ion inertial fusion. The design uses a driver energy of 7 megajoules, which is delivered by 120 beams of singly charged bismuth ions at 3 to 4 gigaelectronvolts. Detailed simulations of the distributed radiator target give an energy gain (ratio of output to input energy) of 57, and the accelerator has a calculated efficiency of 38%. Operating at 6 hertz, the plant has a net

electric power of 1 gigawatt. The final focusing magnets are shielded by a combination of flowing molten salt jets and vortices and solid shielding material, resulting in lifetimes of 30 years or more, based on radiation transport simulations. The superconducting quadrupoles that constitute these final focusing magnets require very large apertures, stored energy, and forces, but magnetic fields of similar magnitude have been achieved in other particle accelerators, proving that the large superconducting magnets required for IFE are indeed possible. The final spot size, which is based on our analytical and numerical understanding of neutralized beam transport, meets the requirements set by the target design. Finally, the current point design is not optimized, but we have identified opportunities in each design area for optimization to improve integrated system performance, reliability, and economics.

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Beam Research Program

The Beam Research Program is focused on two areas: developing high-dose x-ray targets for the DARHT stockpile stewardship facility at Los Alamos National Laboratory, and creating a compact electron accelerator based on dielectric wall technology.

We continued our campaign to develop static x-ray converter targets for the DARHT-2 radiographic accelerator that would be capable of producing four high-dose x-ray pulses over a 2-microsecond interval (DARHT-2 currently produces a microsecond-long electron-beam pulse at about 18 megaelectronvolts and 2 kiloamperes that is chopped into four relatively short pulses). Developing such targets is an extremely challenging task because a single pulse destroys the target, turning it into a plasma. This plasma interacts with the beam on successive pulses, leading to a degradation of the x-ray spot size and a commensurate reduction in x-ray brightness.

We have studied the effects of multiple pulses on x-ray converter targets at the Electron Test Accelerator-II (ETA-II) at Livermore. We used the electron beam from a 1-megaelectronvolt, 2-kiloampere injector to blow up a candidate target and then probed the resulting plasma after an adjustable time delay with the precision beam from ETA-II. The two beams propagated in opposite directions and were brought to a common focus at the target. Our experimental results

indicate that the plasma created from the target provides a source of positive ions that propagate upstream in the electron beam, causing a disruption of the focal spot on a 10-nanosecond timescale. In addition, as the plasma expands with time after the first pulse, the density decreases, which makes x-ray production on the second and subsequent pulses progressively more difficult. We explored a variety of methods to mitigate the effects of beam-plasma interaction and successfully demonstrated, in experiments at ETA-II, novel target designs that increased the confinement time of the targets. Experiments are in progress to verify that these targets will provide substantially improved x-ray conversion efficiencies on the second and subsequent pulses of the electron beam, as required for DARHT.

We continue with research and development of technologies and architectures necessary to greatly reduce the size of a high-current electron accelerator. The basic idea is to replace the typical conducting walls of the accelerator with an insulating wall that can sustain a large tangential electric field (one along the direction necessary for acceleration). Key features of the accelerator include a suitable insulator that can withstand a very high surface-field stress (the dielectric wall), novel pulse forming lines that impress an electric field along the wall, and suitable closing switches that launch the pulses. A candidate material for the dielectric wall, called a high-gradient insulator, consists of finely spaced alternating laminations of conducting and insulating sheets. This configuration has been found to have superior performance to conventional insulators. There is an empirical inverse relationship between the maximum surface-field stress that an insulator can withstand and the applied pulse duration; the highest gradients are achievable with the shortest pulses. We tested a high-gradient insulator consisting of alternating 0.25-millimeter-thick layers of Rexolite and stainless-steel laminations and demonstrated field gradients of 100 megavolts per meter without breakdown for pulses a few nanoseconds in duration (Figure 9). This result is much better than that attained previously with conventional insulators.

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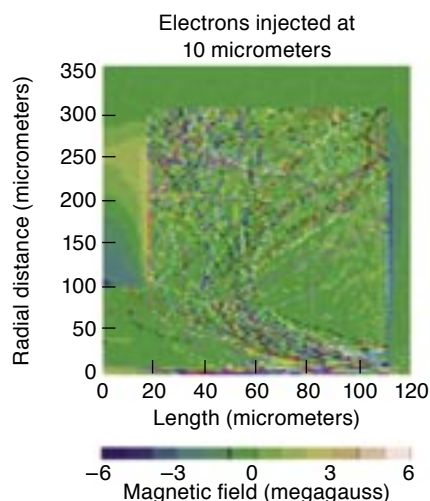
Fast Ignition

Fast ignition offers an alternate approach of energy delivery for inertial confinement fusion

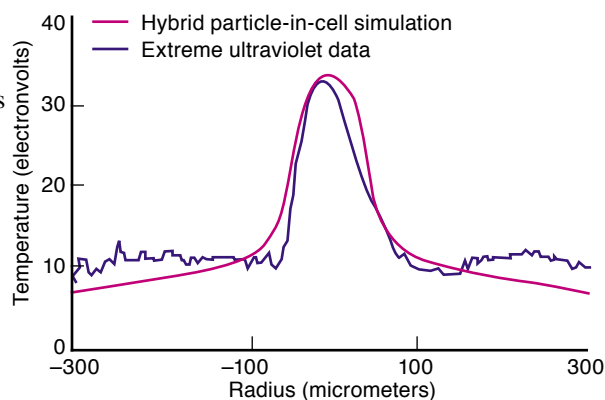
and is applicable to any compression driver, with prospects for higher energy gain, reduced driver energy, and relaxed fuel-compression requirements. The kernel of the concept is fast



9 A close-up of the experimental setup for testing samples of high-gradient insulators. A 3-millimeter-thick, cylindrical sample is placed between two highly polished electrodes. The sample, consisting of alternating 0.25-millimeter-thick layers of Rexolite and stainless steel, withstood 100-megavolt-per-meter gradients without electrical breakdown when subjected to pulses several nanoseconds in duration.



10 Injected electron trajectories in a 100-micrometer-thick slab of solid-density aluminum plasma, as calculated with the hybrid particle-in-cell model (**top**). The spatial variation of the magnetic field outside the slab is also shown. There is good agreement between the calculated and measured temperature profiles at the rear target surface (**bottom**).



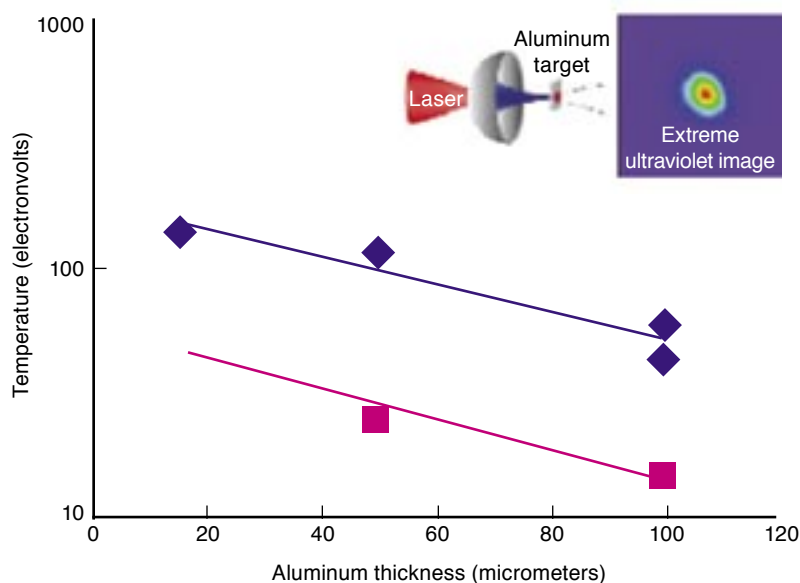
delivery of energy to an ignition hot spot using a short-pulse laser. This may be accomplished through energy transport by either a collimated stream of relativistic electrons or by focused multi-megaelectronvolt protons, both generated with short-pulse laser radiation at high intensity.

We are investigating fast ignition at the concept exploration level through a coordinated program of experiments, theory, and simulation. Experiments are conducted collaboratively at the principal short-pulse laser facilities in Europe and Japan by a team of scientists from Lawrence Livermore, General Atomics, University of California at Davis, Ohio State University, and Princeton Plasma Physics Laboratory. Target design at Livermore is focusing on radiation hydrodynamics simulations of the fuel assembly and concepts for full-scale fast ignition. PIC and hybrid PIC simulations are addressing the difficult problems of relativistic laser-plasma interactions and transport of energy by electrons and protons. The goal of these efforts is to benchmark the PIC and hybrid PIC modeling against experiments,

and integrate the codes to a level that will enable complete design of both proof-of-principle and full-scale fast-ignition experiments at the National Ignition Facility and elsewhere.

Understanding the transport of relativistic electrons produced in the short-pulse laser-plasma interaction is key to predicting the performance of fast ignition. We have investigated electron transport and isochoric heating through computational models and experiments. Our principal theoretical accomplishment has been development of a hybrid PIC code (based on an adaptation of the Large-Scale Plasma code) for modeling transport of high current-density relativistic electrons in dense matter. The required electron source is obtained from PIC simulations of the focused laser beam interacting with preformed plasma. In experiments at the Vulcan laser at the Rutherford Appleton Laboratory in the United Kingdom, we have used both imaging of the K-alpha fluorescence and thermal extreme-ultraviolet emission as diagnostics of electron flux and heating in several target geometries [*Physical*

11 Schematic of the proton focusing and heating experiment (**top middle**), and data showing the extreme ultraviolet image (**top right**) of the heated region with a diameter of 90 micrometers (full width at half maximum). Plot shows peak temperatures at the rear surface of aluminum targets of various thicknesses obtained for heating by protons (diamonds) and electrons (squares), using the Vulcan petawatt laser to irradiate the target.



Review E **69**, 066414 (2004)]. We have obtained experimental data for the spatial and angular pattern of transport and for heating in solid materials, in fast ignition cones, and most recently in imploded matter. The data for isochoric heating of a slab target provided the first reasonable benchmark of the hybrid PIC model (Figure 10).

The ballistic focusing of laser-generated protons offers another approach to isochoric heating for fast ignition. This concept originated from research at the world's first petawatt laser at Lawrence Livermore [*Physical Review Letters* **86**, 436 (2001)]. The first demonstration of such focusing and heating using a hemispherical shell target as the proton source occurred at the JanUSP laser at Livermore [*Physical Review Letters* **91**, 125004 (2003)]. We carried this investigation forward to larger-scale experiments at two petawatt laser facilities, Gekko in Japan and Vulcan in the United Kingdom. Using our extreme ultraviolet diagnostic of isochoric heating developed for the earlier electron transport studies, we demonstrated that protons could heat through 100 micrometers of solid aluminum, raising the temperature of a 100-micrometer-diameter region to about 100 electronvolts (Figure 11). Also notable is that this temperature was more than three times higher than that produced by electron heating using the same laser pulse focused on the front surface of the aluminum target. Work is continuing to develop a predictive model and to assess the feasibility of fast ignition using proton heating.

The fast ignition approach to inertial confinement fusion has the advantage that no hot spot need be formed by the implosion. The "cone-focused" concept takes advantage of low symmetry requirements to hold open a clear path for the ignition laser so that it can generate hot electrons very close to the imploded, high-density fuel. The initial capsule has a conical shell of dense material penetrating through one side to near the capsule center. This design, invented and refined at Livermore, has shown

sufficient promise that experiments are now being conducted around the world to explore this target configuration [*Physics of Plasmas* **10**, 1925 (2003)]. We collaborated with researchers at General Atomics, the Laboratory for Laser Energetics at the University of Rochester, and the Institute of Laser Engineering at Osaka University in Japan to verify the hydrodynamics of cone focusing on the Omega laser at the Laboratory for Laser Energetics. We conducted several series of cone-focused implosion experiments on plastic capsules, both indirectly and directly driven. Radiographs of implosions showed dense cores similar to those predicted in our calculations.

We have also designed integrated, proof-of-principle tests of the cone-focused fast ignition concept at the National Ignition Facility. These experiments would use a cone-focused implosion of a noncryogenic deuterated plastic shell, deposition of short-pulse laser energy into the cone tip, and K-alpha fluorescence diagnosis of the hot-electron coupling to the imploded core. With 250 kilojoules of laser drive for the implosion (provided by four laser beams of the National Ignition Facility bundled together), the capsule can be imploded to a dense plasma. Then one short-pulse beamlet shot into the cone will answer three important questions:

- How many hot electrons were generated?
- Where did the electrons deposit their energy?
- How much energy was deposited in the core?

We expect one beamlet to generate several hundred joules of hot electrons that will excite K-alpha line emission from the zirconium dopant in the capsule, in amounts directly proportional to the energy deposition. The high electrical conductivity conditions in the imploded core are sufficiently similar to those expected for IFE capsules, so that the results should scale and be useful as a benchmark test of our integrated simulation of such targets.

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The Presidential

Science Awards

Awards

PHYSICS AND ADVANCED TECHNOLOGIES AWARDS

FELLOWSHIPS

American Physical Society

The American Physical Society (APS) Fellowship recognizes those members who have made significant advances in knowledge through original research or who have made significant, innovative contributions in the application of physics to science and technology. The APS may also recognize members who have made significant contributions to the teaching of physics or to the activities of the society. Each year, no more than one-half of one percent of the current APS membership is elected to the status of fellow. The 100-year-old society numbers over 40,000 physicists worldwide. During 2002 and 2003, five physicists from PAT were named APS fellows for their outstanding contributions to physics.



Yu-Jiuan Chen of the Fusion Energy Program, elected in November 2002, was cited for her work in revolutionizing the achievable beam quality of linear induction accelerators and advancing the state-of-the-art of flash x-ray radiographic technology.



Forrest Rogers, a physicist in V Division who has worked at the Laboratory for more than 30 years, was also elected in November 2002. Rogers was cited for developing the ACTEX equation-of-state and OPAL opacity models and applying them to a range of astrophysical and laboratory plasma problems including helioseismology, variable stars, and laser shock experiments.



Andrew McMahan, a physicist in H Division for 28 years, was elected a fellow in 2002 for pioneering work in the computation of effective Hamiltonian parameters for the superconducting copper oxides and phase transitions of materials under high pressure, and the subsequent solution of the associated models. He was nominated for fellowship by the Computational Physics Division of the APS.



Giulia Galli, who leads the Quantum Simulations Group in H Division, was elected in December 2003. She was cited for her important contributions to the field of ab initio molecular dynamics and to the understanding of amorphous and liquid semiconductors and quantum systems. She conducts computational research in condensed matter and materials physics.



Erich Ormand, acting group leader for Nuclear Theory and Modeling in N Division, was elected in December 2003 for his important contributions to nuclear structure physics, including both the ab initio shell-model calculations and the Monte Carlo approach, and for his contributions to nuclear physics as applied to stockpile stewardship. He conducts research in nuclear structure theory and nuclear reaction modeling.



Steven Hatchett, a plasma physicist in the AX Division of the Defense and Nuclear Technologies Directorate (who has also worked in the Fusion Energy Program in PAT) was elected fellow in 2003. He was recognized

for contributions to theory and experiments of implosion physics for inertial confinement fusion and for innovative designs for fast ignition. He was nominated for fellowship by the Plasma Physics Division of the APS.



American Academy of Arts and Sciences

Claire Max, founding director of PAT's Institute of Geophysics and Planetary Physics, joined Edward Teller in 2002 as the only other Livermore employee to be named a

fellow of physics by the American Academy of Arts and Sciences. The academy was founded

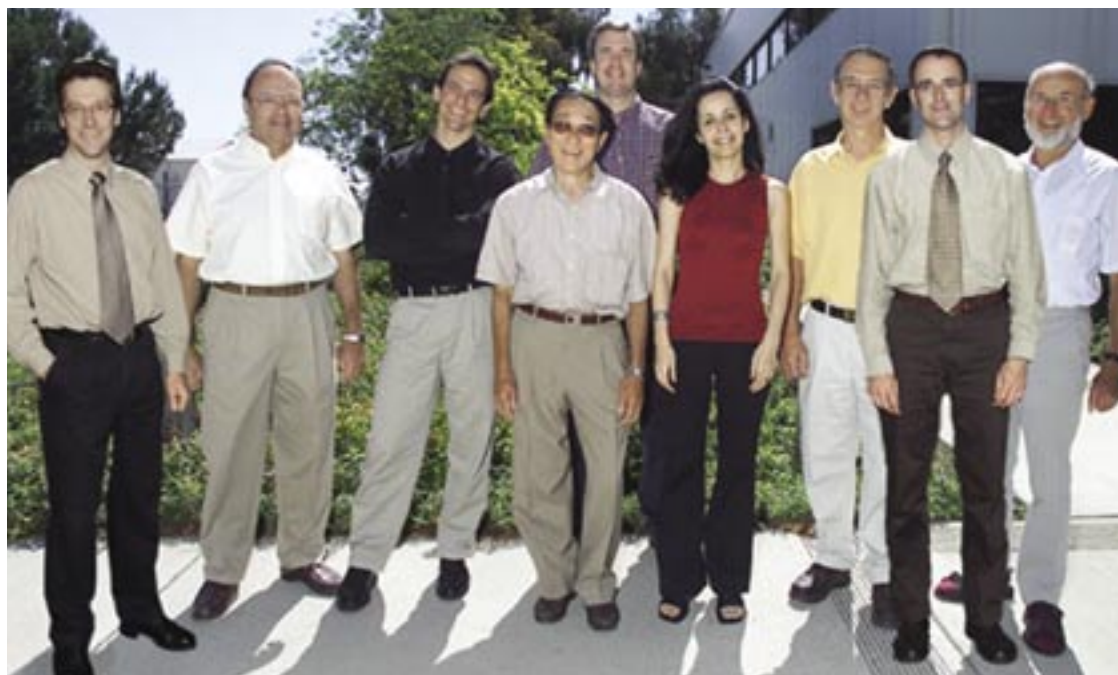
during the American Revolution by John Adams and other leaders to provide a forum for a select group of scholars, government officials, and business leaders to work together on behalf of the democratic interests of the republic. Max's recent work focuses on the use of adaptive optics on telescopes at the Keck Observatory. Through adaptive optics, the resolution of fine details of astronomical objects is greatly increased. Installed in 1999, the Keck adaptive optics system has enabled astronomers to minimize the blurring effects of the Earth's atmosphere, producing images with unprecedented detail and resolution. Astronomers are obtaining infrared images with four times better resolution than the Hubble Space Telescope, which orbits high above the Earth's atmosphere.

AWARDS

R&D 100 Awards

Researchers from Lawrence Livermore and Veeco Instruments Inc. teamed to develop a fundamental technology for high-volume manufacturing of the next generation of computer chips, which won a 2002 R&D 100

Richard Levesque (second from left), Regina Soufli (fourth from right), and Eberhard Spiller (far right) from I Division were part of the Livermore team that worked with private industry to develop the Production-Scale Thin Film Coating Tool, a highly precise deposition system that opens the door to advanced, high-volume manufacturing of the next generation of microprocessors. Other members from the Livermore team pictured include (left to right) Jim Folta, Claude Montcalm, Swie-In Tan, Mark Schmidt, Fred Grabner, and Chris Walton.



Award. **Regina Soufli, Steve Vernon, Richard Levesque, and Eberhard Spiller** from I Division were part of the Livermore team that help develop the Production-Scale Thin Film Coating Tool, which will lead to computer chips 100 times faster and with 1000 times more memory than those currently available. The coating tool is the only deposition system able to apply multilayer coating thicknesses to within a quarter of an atom.

STIM-2002, a miniaturized medical device that delivers low-level electrical pulses through the skin to inhibit pain signals to the brain, also won a 2002 R&D 100 Award. **Bill Colston** from M Division was part of the Livermore Medical Technology Program team that collaborated with Florida-based Cyclotec Advanced Medical Technologies and the Biophysical Laboratory of Sarov, Russia, on developing the wireless, inexpensive module. The device is worn like a bandage and provides rapid pain relief for millions with injuries or arthritis or who are recovering from surgery.

The Extreme Ultraviolet Lithography Full-Field Step-Scan System represents a

revolutionary lithography breakthrough, enabling microprocessors that are 10 times faster with active transistors and memory chips that can store 40 times more information. This system was honored with both a 2003 R&D 100 Award and one of three “Editor’s Choice” awards for the most outstanding achievement among the award winners. **Don Sweeney, Regina Soufli, Henry Chapman, Richard Levesque, Nhan Nguyen, Donald Phillion, Michael Johnson, Gary Sommargren, and Eberhard Spiller** of I Division were part of a collaboration involving Lawrence Livermore, Lawrence Berkeley, and Sandia national laboratories, known as the Virtual National Laboratory, that developed the technology. The team was honored for making the “greatest improvement upon an existing technology” in advancing the field of lithography.

Scot Olivier and Abdul Awwal of I Division were part of a six-institution team that pioneered a technology to enhance vision and improve the early diagnosis and treatment of retinal diseases, which also won a 2003 R&D 100 Award.



Bill Colston (left) displays an application of the STIM-2002, a medical device that uses transcutaneous electrical nerve stimulation to combat pain. Also shown are Alexander Rubenchik (center) and John Marion from Lawrence Livermore.

Known as the Micro-Electrical-Mechanical Systems-Based Adaptive Optics Phoropter, this breakthrough utilizes advances from adaptive optics technology, also used for the world's largest telescopes and micromachining. It is anticipated that the new phoropter may one day allow clinicians to measure and apply the proper corrections, then allow patients to immediately see the actual improvements in their quality of vision and offer feedback.

Eberhard Spiller from I Division (a former staff member and current participating guest) was a member of the team that developed the Ion Beam Thin Film Planarization process, which won a third 2003 R&D 100 Award for the Laboratory. It is used in an effort to produce nearly defect-free masks for extreme ultraviolet lithography (EUVL) of computer chips. The process uses a thin film coating and ion-beam etching technique to generate nearly perfect surfaces. Work for this effort was funded under the Department of Energy's largest-ever cooperative research and development agreement (the EUVL CRADA) involving three national laboratories, Intel, and five other companies.



American Physical Society's John Wheatley Award

PAT physicist **Kennedy Reed** was named the 2003 recipient of the American Physical Society's John Wheatley Award. The award is given every

two years to a physicist who, working in a developing country, has made an outstanding contribution to the development of physics in that region by working with local physicists in research or teaching. Reed was cited for his multifaceted contributions to the promotion of physics research and education in Africa, for developing agreements for exchange of faculty and students between US and African institutions, for organizing and conducting international workshops and conferences on physics in Africa, and for advocating increased US and international involvement with physics in Africa. In addition to his atomic physics research in V Division, Reed is director of the Research Collaborations Program for Historically Black Colleges and Universities and Minority

Livermore team members for the Extreme Ultraviolet Lithography Full-Field Step-Scan System, the first tool that demonstrates all of the key technologies needed for production of next-generation microprocessors (standing, from left): Eberhard Spiller, Russ Hudyma, Rick Levesque, Chris Walton, Regina Soufli, John Taylor, Sherry Baker, Mark Schmidt, Franklyn Snell, Layton Hale, Michael Johnson, Nhan Nguyen, Don Phillion, Henry Chapman, and Butch Bradsher; (kneeling): Gary Sommargren, Ken Blaedel, Jim Folta, and Don Sweeney.



Institutions, which is within the Laboratory's University Relations Program.



**American Society for
Precision Engineering
Lifetime Achievement
Award**

Optical physicist **Gary Sommargren** received a Lifetime Achievement Award in October 2003 from the American Society

for Precision Engineering, in recognition of his contributions to the science of precision optical metrology. Sommargren is the inventor of the heterodyne optical profiler, used for measuring the surface roughness of optical surfaces to the sub-nanometer level. He also invented and developed a phase-shifting diffraction interferometer, which is a key technology advance for the success of EUVL tools, and has applied this technology to the development of astronomical telescopes at the Center for Adaptive Optics at the University of California (UC) at Santa Cruz.

**Presidential Early Career Award for Scientists
and Engineers**

The Presidential Early Career Award is one of the nation's highest honors, recognizing scientists and engineers at the onset of their research career. **Mark Herrmann**, a plasma physicist in AX Division in the Defense and Nuclear Technologies Directorate and who has also worked in PAT's Fusion Energy Program, was one of 60 professionals nationwide to receive the award in 2002. Simultaneously, he also received an Early



Livermore members of the Micro-Electrical-Mechanical Systems-Based Adaptive Optics Phoropter team included I Division's Scot Olivier (left) and Abdul Awwal (second from right), along with Steve Jones, Kevin O'Brien, Don Gavel (center, left to right), and Brian Bauman (far right). The new optical device promises to greatly improve the process of determining the necessary correction for eyeglasses and contact lenses.

Career Award from the Department of Energy for his work elucidating the requirements for ignition in inertial confinement fusion targets.



American Physical Society Nicholas Metropolis Award

Physicist **John Pask**, who joined H Division in late 2001, was the recipient of the American Physical Society Nicholas Metropolis Award in 2001 for outstanding doctoral thesis work in

computational physics at UC Davis. He was cited for contributions that included formulating and implementing a new finite-element-based method for solving equations of the density functional theory. Currently, he conducts computational research in condensed matter and materials physics.

Alameda County Women's Hall of Fame

Claire Max was recognized for her contributions to science during the 10th Annual Alameda County Women's Hall of Fame Awards ceremony in March 2003. Max has had a successful career at Lawrence Livermore, joining as a physicist in 1974. In the early years, she worked on laser plasma interactions within the Inertial Confinement Fusion Program. In 1984, she was named as the director of the Institute of Geophysics and Planetary Physics; in 1993, as director of Institutes in the then-named Physical Sciences Directorate; and in 1995, as director of University Relations. Max now serves as associate director for the National Science Foundation's Center for Adaptive Optics at UC Santa Cruz, in which the Laboratory plays a significant role, and pursues her astronomy research at PAT's Institute of Geophysics and Planetary Physics.

Federal Laboratory Consortium Award for Excellence in Technology Transfer

Started in 1974, the Federal Laboratory Consortium Award for Excellence in Technology Transfer recognizes individuals and teams at federal laboratories for uncommon creativity and initiative in transferring to the private sector an advanced technology that significantly benefits

industry, state and local governments, and/or the general public. More than 650 federal government laboratories and research centers compete for the award.

The Virtual National Laboratory for extreme ultraviolet lithography—a consortium of Lawrence Livermore, Lawrence Berkeley, and Sandia (Livermore) national laboratories—received the 2003 award for transferring technology to industry that will lead to more powerful microprocessors and memory chips with increased storage capacity. The collaboration developed the next-generation lithography, which overcame the limitations of current technology by using coated mirrors, rather than lenses, to bend and focus the shorter-wavelength light needed to print integrated circuits with smaller features on semiconductor wafers. The technology and associated knowledge were transferred to an industry consortium whose members included Micro Devices, IBM, Infineon, Intel, Micron Technologies, and Motorola. Scientists and engineers in I Division have been key members of the Livermore team participating in the Virtual National Laboratory and have made many important contributions to the success of the EUVL program.

Weapons Recognition of Excellence Awards (2001–2002)

Livermore's Defense and Nuclear Technologies Directorate, the National Nuclear Security Administration, and the Department of Energy present Weapons Recognition of Excellence Awards annually to recognize people who have contributed significant accomplishments to the Stockpile Stewardship Program. **Art Toor**, retired from V Division, and **David Reisman**, now in Defense and Nuclear Technologies' B Program, were members of a multilaboratory team honored with a 2001 award for developing isentropic compression experimental techniques and applying them to improve understanding of stockpile materials properties. The technique, demonstrated at the Z accelerator at Sandia National Laboratories, uses high currents and magnetic fields to achieve shockless compression of materials to megabar pressures over time

intervals of 200 to 300 nanoseconds. This provides a new ability to study stockpile materials with high accuracy at pressures appropriate to weapon conditions. Other members of the team included personnel from Sandia and Bechtel Nevada.

Deborah Brown, George Caporaso, Frank Chambers, Yu-Jiuan Chen, Karen Houston-Patterson, Marlene Leon, John Weir, and Glen Westenskow from the Beam Research Program in PAT were members of a multilaboratory team recognized with a 2002 award for developing the second beamline of DARHT, an important stockpile stewardship facility at Los Alamos National Laboratory. DARHT is a dual-axis, x-ray radiographic machine that, when fully operational, will provide advanced imaging capability for hydrodynamic tests of weapon assemblies using surrogates for fissile materials.

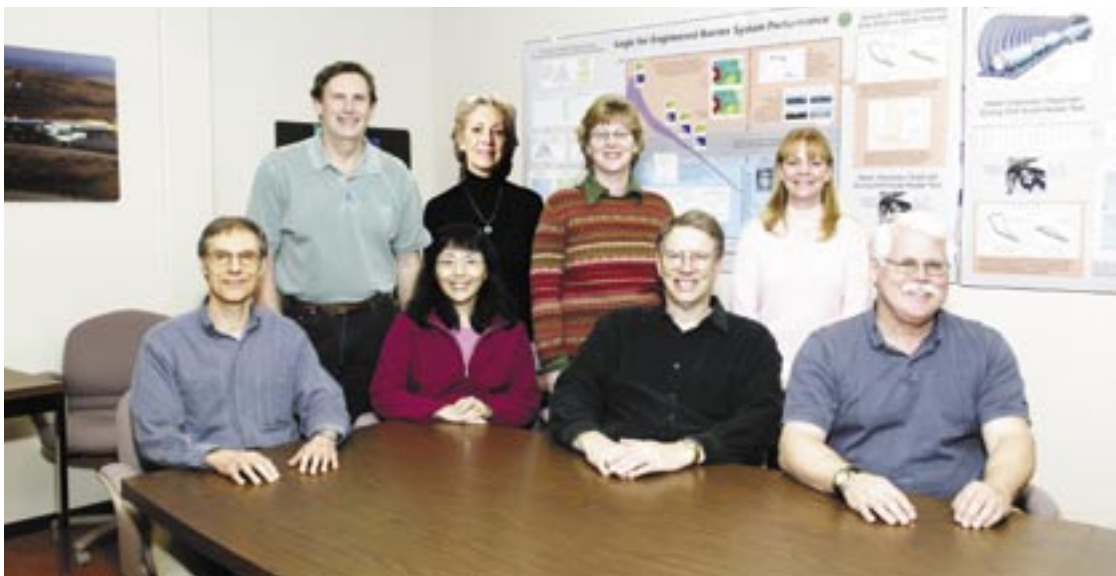
Laboratory Science and Technology Awards

The Laboratory Science and Technology awards were established in 2000 and are given annually by Livermore's director for notable achievements in science and technology. **Doug Wright** of N Division and his team from the High Energy Physics and Accelerator Technology Group earned a 2002 award for their work searching for the origin of the universe.

The team, which included **Richard Bionta** of I Division, **David Lange** and **Marshall Mugge** of N Division, and **Karl van Bibber** of the PAT associate director's office, was part of a large international collaboration that studied the existence of CP violation—a fundamental process that favors particles over antiparticles—at the B-Factory of the Stanford



Doug Wright, David Lange, Karl van Bibber, and Marshall Mugge (left to right) stand in front of the accelerator and detector facility known as BaBar, which is used to measure the production and decay of subatomic particles. Information from these experiments could help solve crucial problems in particle physics as well as provide information on the nature of the universe. (Background photo courtesy of Stanford Linear Accelerator Center.)



Livermore members of a multilaboratory team that developed the second beamline of DARHT, an important stockpile stewardship facility that will provide advanced imaging for tests of weapon assemblies (seated, from left): George Caporaso, Yu-Jiuan Chen, Frank Chambers, and John Weir; (standing, from left): Glen Westenskow, Karen Houston-Patterson, Marlene Leon, and Deborah Brown.

Linear Accelerator Center. For 40 years prior to the discovery of CP violation in the B-Factory system, only one CP-violating process had ever been observed.



**Plasma Physics
Distinguished Lecturer**
The American Physical Society Division of Plasma Physics named physicist **Steve Allen** of PAT's Fusion Energy Program to their Distinguished Lecturer's Program for

2002–2003. As one of six lecturers chosen nationwide, he traveled to US colleges and universities throughout the year to discuss his work in plasma physics with students and faculty. Allen is the program leader for the Laboratory team working on the DIII-D tokamak, a collaborative effort between Lawrence Livermore and General Atomics in San Diego.

Physics Excellence by the Numbers

Category	2002*	2003*
Significant awards	4	8
R&D 100 and Federal Laboratory Consortium awards [†]	2	4
Society fellowships	3	2
Total fellows	44	46
Published refereed journal articles	>150	430
Published conference proceedings	>128	177
Invited talks	N/A**	231
Patents issued	30	24
Patent applications	17	20
Invention disclosures	15	19
Royalty revenue (\$M) ^{††}	1.32	0.5
Newly executed licenses	5	8

* Data for 12 months ending May 31, except as noted below.

[†] Calendar year.

** Data not available.

^{††} Fiscal year ending September 30.

ABOUT THE BACK COVER

Top: Students from the Research Collaborations Program for Historically Black Colleges and Universities and Minority Institutions analyzing data at the Livermore Electron Beam Ion Trap facility. The students participated in a workshop on astrophysical spectra sponsored by the National Aeronautics and Space Administration, which exposed the students to astrophysical observations, atomic physics, experimental techniques, and data analysis.

Middle: Image of the human retina showing how adaptive optics in an ophthalmic imaging instrument can give an unprecedented, cellular-level view. Livermore is part of a team led by the University of Rochester, which is developing such instruments under sponsorship of the Department of Energy's Bioengineering Research Partnership Program.

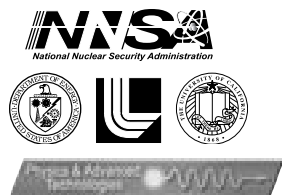
Bottom: Three-dimensional simulation of turbulence in the boundary plasma of a tokamak magnetic fusion energy device. Shown is the spatial (vertical) and temporal (horizontal) distribution of density fluctuations in the outer midplane of the device calculated with the Livermore-developed BOUT code. Lower half of the image corresponds to the edge plasma.



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